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Title: LANL Fuel Cell Program Overview

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Intended for: Slides for distribution to Chemours

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Los Alamos NATIONAL LABORATORY

LANL Fuel Cell Program

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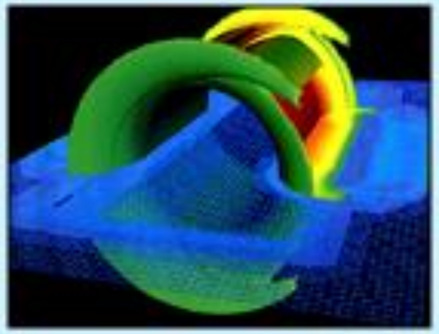
LA-UR-21-25696

Mission

LANL Mission: National Security Science

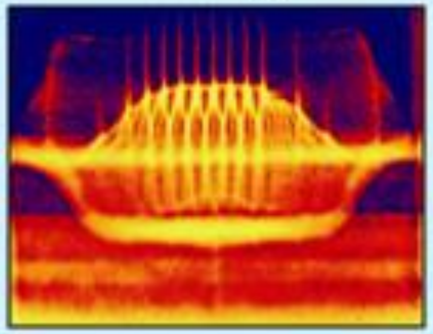
Stockpile Stewardship



Large-Scale Simulation

Stockpile Stewardship

B61-7/11 Strategic Bomb



Proton radiography

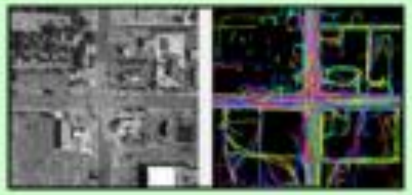
Pit Manufacturing

W76, W78, W88 for Trident & Minuteman III

*W-93

Global Security

Non Proliferation



Intelligence Analysis

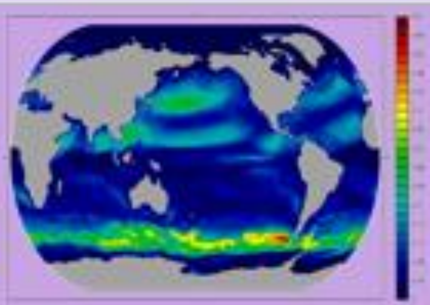
Space Systems

Six other product lines

Energy Security

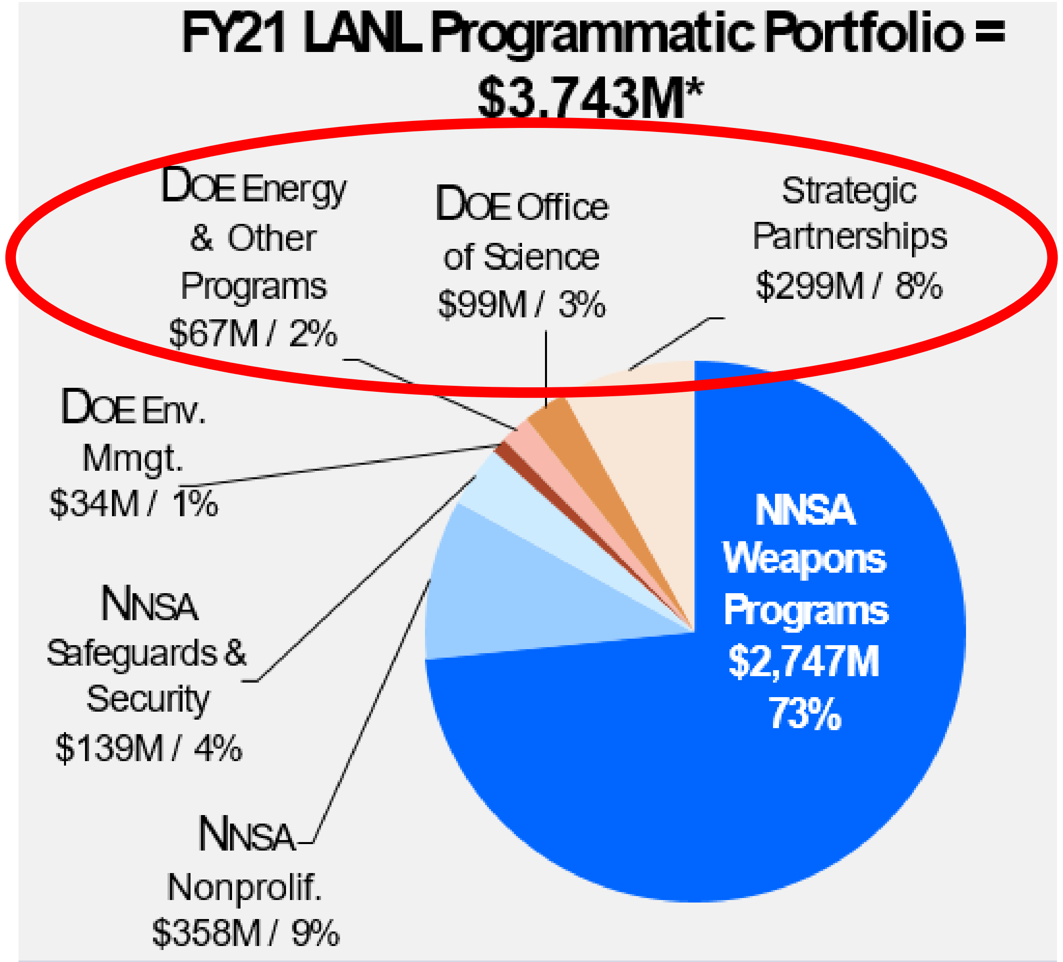
Materials and Concepts for Clean Energy

Nuclear Energy



Climate Energy Nexus

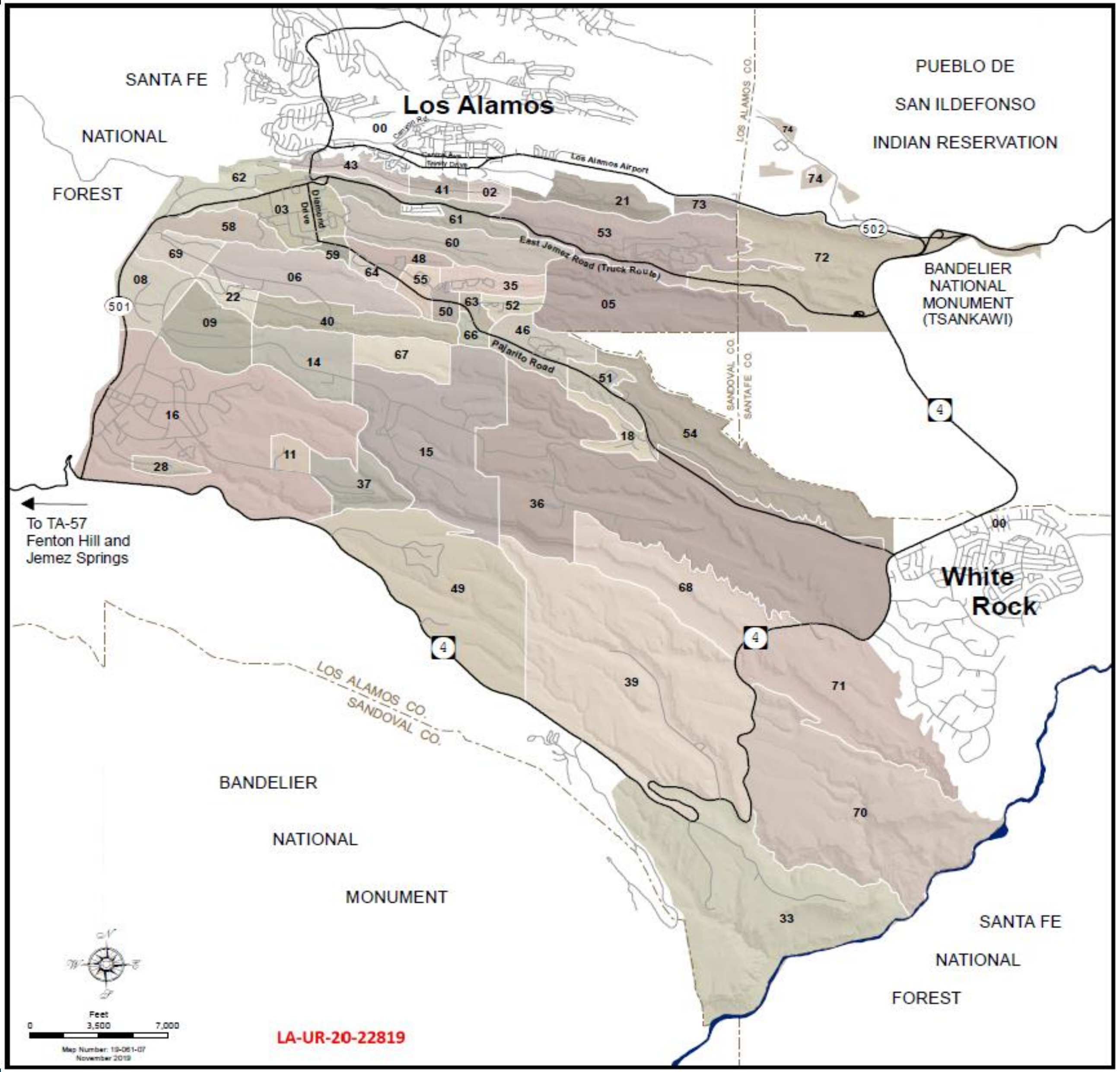
Our national security mission is broad and important
— and is motivated and enabled by ST&E discovery



LANL STATISTICS	
40 square miles	1,280 bldgs., 9M sq ft
47 technical areas	11 nuclear facilities
13,000 workers on site	8,900 career employees
1,144 students	498 postdocs
Average employee age: 43	65% male; 35% female 45% minorities

***FY22 Budget is ~ 4.1M**
****FY23 Presidents Request calls for $1B increase**

LANL covers 40 square miles, 47 technical areas (TA's) → The size of Washington D.C.

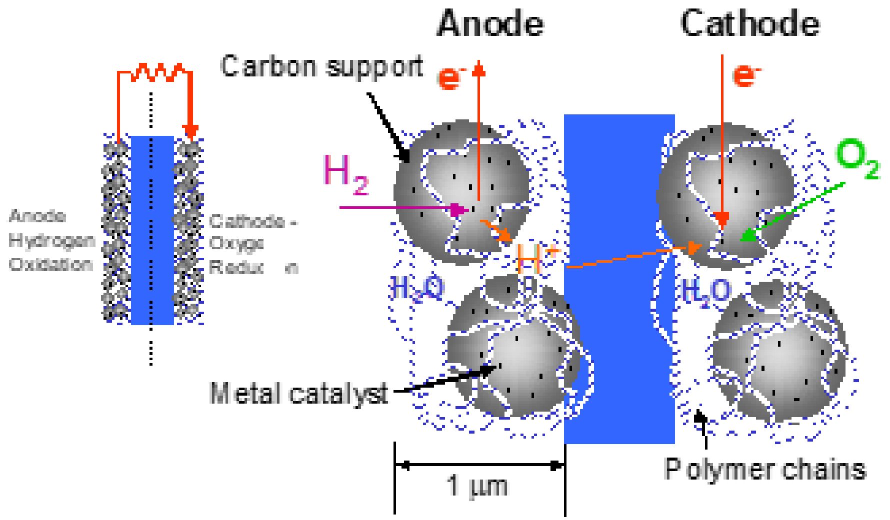


- Approximately 60% of the LANL workforce lives outside Los Alamos County
- Increased use of bussing and alternative transit options will reduce overall congestion
- Commuter bussing solutions also offer an opportunity to reduce greenhouse gases
- LANL is exploring incentives to increase participation in mass transit options to achieve 2500 trips per day
- Mass transit options will require offsite parking and bussing service with either express busses or increased public mass transit
- Supports near future electrification (hydrogen and/or battery) of the bus fleet(s) to create a sustainable commuting solution

Fuel Cell R&D at Los Alamos
Breakthrough MEA: Membrane Electrode Assembly

- longest running non-weapons programs at LANL (since 1977)
  - **The first fuel cells for transportation program**
- The current DOE HFTO program grew out of the Los Alamos program
- Primarily polymer electrolyte membrane (PEM) technology
- Cost and durability are biggest barriers to commercialization
- Program focus is obtaining fundamental understanding to enable "knowledge-based innovation," and subsequent materials and process development

LANL Enabling Breakthrough Thin Film Electrode



An electrochemically active reaction site must have reactant access to catalyst, available electronic and ionic conduction paths, and manage water

US Patents #4,876,115, #5,211,984 and #5,234,777

→ Every Fuel Cell Vehicle relies on technology developed at LANL

LANL Program: Materials Emphasis

- LANL Leads Projects That Focus on Performance, Cost and Durability
  - M2FCT (Million Mile Fuel Cell Truck)
    - FC-PAD Consortia (Fuel Cell Performance and Durability)
  - ElectroCat 2.0 Consortia (PGM-free electrocatalysis)
  - Low-PGM Electrocatalysis
  - MEA Design (Membrane Electrode Assembly) – Low PGM, PGM-Free
  - Alternative membranes
    - High Temperature polymer
    - Intermediate Temperature Proton Conductors
    - Alkaline
  - Impurity effects on fuel cell performance
  - Water transport
  - Alternative Fuel Cells:
    - Direct fuel: methanol (DMFC) and DiMethylEther (DDMEFC)
  - Hydrogen Safety Codes & standards; sensors; fuel quality
  - Water Electrolysis
  - Energy Storage (Flow Batteries/Flow Cells)

Strong record of national and international collaborations with other labs, academia, and industry

Rodney Borup (co-lead with LBNL)
Million Mile Fuel Cell Truck (M2FCT)

- Enhancing the performance and durability of polymer electrolyte membrane fuel cells while simultaneously reducing their cost
- Demonstrate world-class improvements in fuel cell performance and durability that exceed the targets set by the U.S. DOE
- International collaborations: EU funded IMMORTAL, ID-FAST, Japan FC-CUBIC

Piotr Zelenay (co-lead with ANL)
ElectroCat 2.0: Energy Materials Network Consortium

- Accelerating development and deployment of platinum group metal-free electrocatalysts in fuel cells and electrolyzers
- Systematic approach combining experiment, theory, machine learning (ML), high-throughput and combinatorial techniques, advanced materials characterization
- International collaborations: PEGASUS, CRESCENDO, IFCC, universities (including in France, Germany, Israel, Italy, Poland)

BERKELEY LAB Lawrence Berkeley National Laboratory
OAK RIDGE National Laboratory
Pacific Northwest NATIONAL LABORATORY
Carnegie Mellon University
NIKOLA MOTOR COMPANY
BROOKHAVEN NATIONAL LABORATORY
gm
Argonne NATIONAL LABORATORY
THE UNIVERSITY OF TENNESSEE KNOXVILLE
NREL NATIONAL RENEWABLE ENERGY LABORATORY
TECHNISCHE UNIVERSITÄT DARMSTADT
CRESCENDO
IFCC Israeli Fuel Cells Consortium
PEGASUS PGM Free Catalyst

M2FCT Partners: National Labs, Universities, Industry

"Team-of-teams" approach for rapid feedback, idea development, information exchange, resulting in an effort that is more than the sum of its parts

MEA Projects
gm · Carnegie Mellon University · NIKOLA

Membrane Projects
University of Tennessee · Lubrizol · 3M · NIKOLA

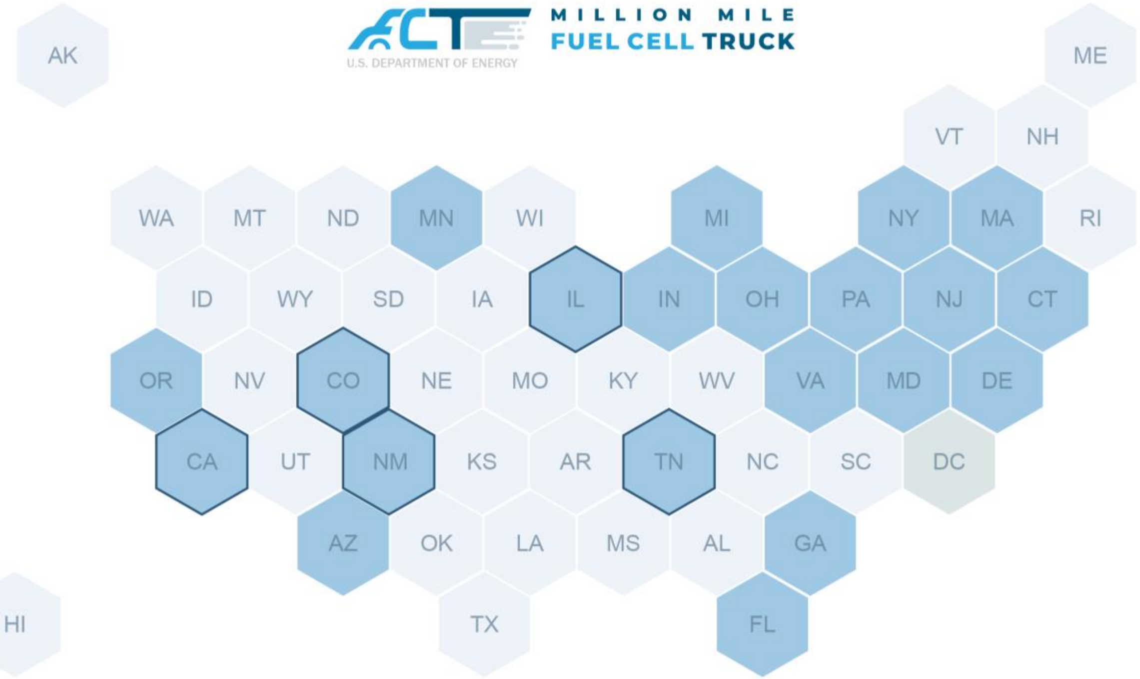
Stack Projects
Cummins · PLUG POWER

Bipolar Plate Projects
Raytheon Technologies · NEOGRAF SOLUTIONS · TreadStone Technologies, Inc. · gm · PLUG POWER

Air Management Projects
CATERPILLAR · EATON · R&D Dynamics Corporation · MAHLE Driven by performance

MILLION MILE FUEL CELL TRUCK

U.S. DEPARTMENT OF ENERGY



LABS	ACADEMIA		INDUSTRY	
Primary Labs	**Partners**		**Partners**	
LANL	Cornell	Northeastern	3M Company	Lubrizol
LBNL	Carneige Mellon Univ.	UC Irvine	Akron Polymer Products	Mahle
ANL	Colorado School of Mines	UC Merced	Ballard	Nikola Motors
NREL	Drexel University	University at Buffalo	Chemours	Pajarito Powder
ORNL	Florida International Univ.	University of Tennessee	Cummins	Plug Power
Partners	GeorgiaTech		Caterpillar	NeoGraf Solutions
PNNL			Eaton	R&D Dynamics Corp
BNL			General Motors	Raytheon Technologies
NIST			Kodak	Strategic Analysis
				TreadStone Technologies

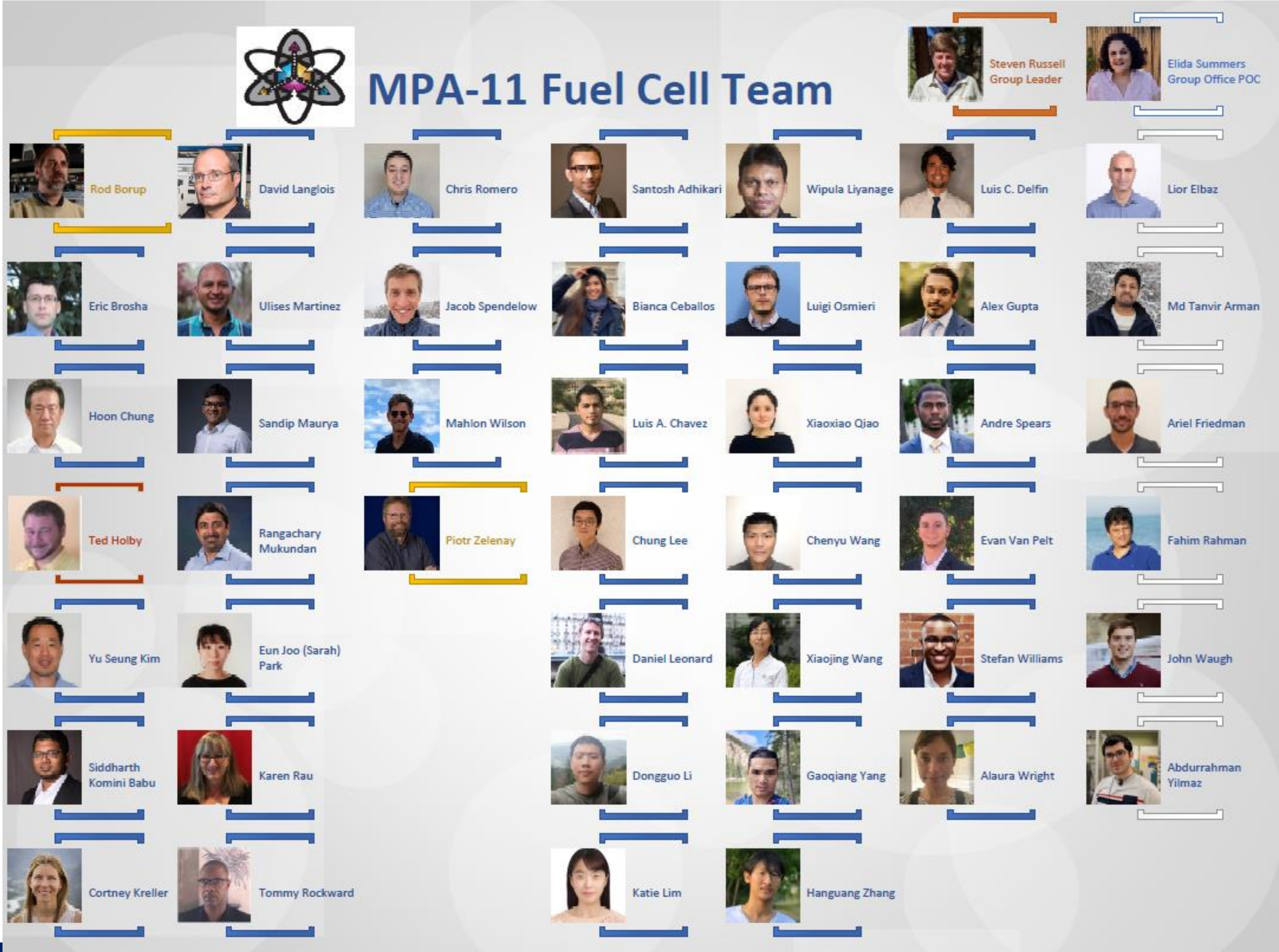
Main Laboratories
Los Alamos National Laboratory · Berkeley Lab · Argonne National Laboratory · Oak Ridge National Laboratory · NREL National Renewable Energy Laboratory

Affiliate Laboratories
Pacific Northwest National Laboratory · NIST National Institute of Standards and Technology · Brookhaven National Laboratory

Discretionary Funds Project Partners
Drexel University · University of California Merced · Buffalo State The State University of New York · FIU Florida International University · UCI

Fuel Cell People

- **Expertise from Chem. Eng., Chemistry, Material Sci., Mech. Eng. & Physics**
- **Scientists with over 200 years of experience fuels cells and over 25 Ph.D.'s**



People

Fuel Cell Program has an extensive record of students and post-docs

Funding

- DOE EERE HFTO
- (Energy Efficiency and Renewable Energy – Hydrogen Fuel Cell Technologies Office)
- NNSA
- ARPA-E
- CRADAs
- LDRD
- OE
- BES

Ultimate Objective is Process-Performance Optimization

Critical Material Attributes (CMA)

- Moisture
- Particle Size
- Age
- Purity
- Shelf-life
- Storage Conditions
- Crystallinity

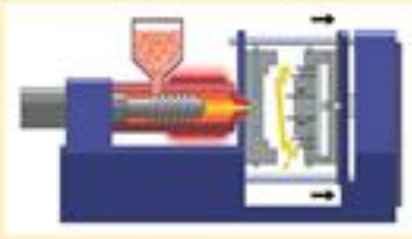
In progress

Examples only

Critical Processing Parameters (CPP)

- Composition
- Melting Temp
- Cylinder Temp
- Mold Temp
- Injection Pressure
- Injection Speed
- Time (molding cycle)
- Viscosity
- Fill Time

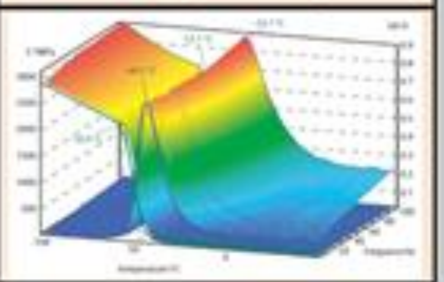
Examples only



Critical Quality Attributes (CQA)

- Hardness
- Density
- Residual Stresses
- Outgassing
- Thickness
- Shrinkage
- Time (molding cycle)
- Viscoelastic
- Bonding/Strength
- Homogeneity
- Crack resistance

Examples only



Critical Performance Attributes (CPA)

- Aging
- Compatibility
- Performance
- Etc..

Examples only

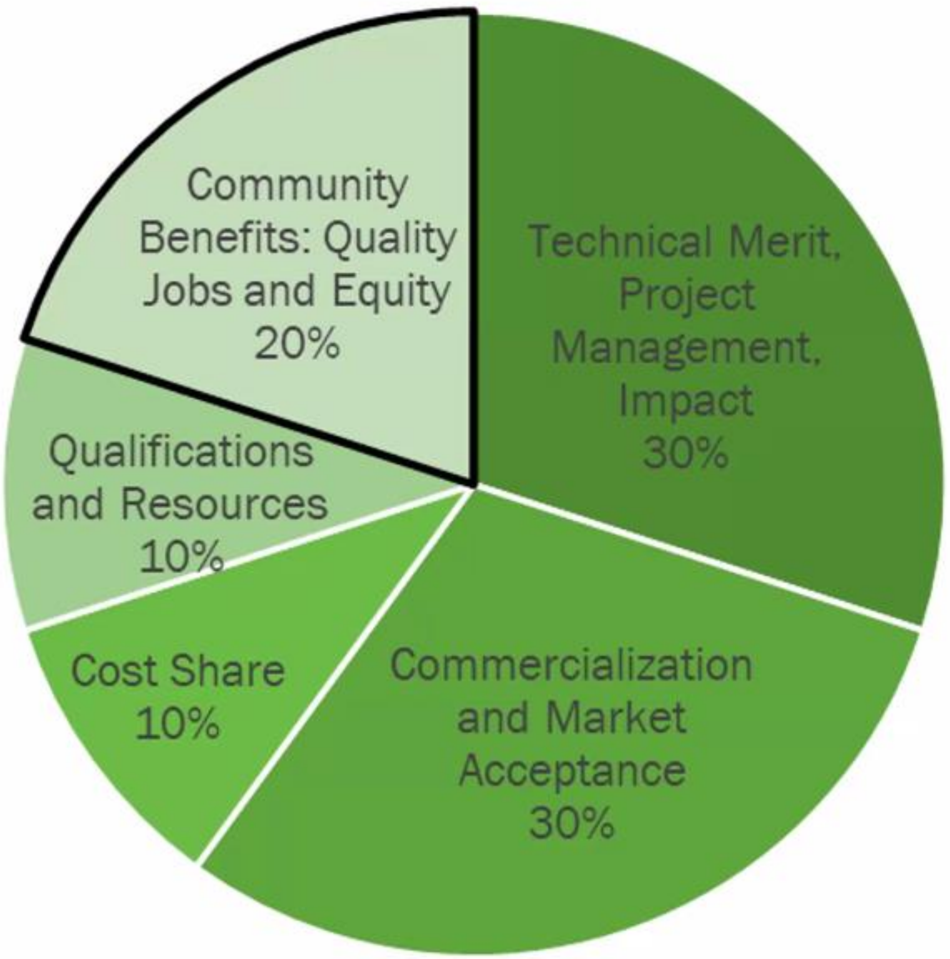
Building Good Jobs and Equity into our work

Department of Energy

Biden Administration Announces $3.16 Billion from Bipartisan Infrastructure Law to Boost Domestic Battery Manufacturing and Supply Chains

MAY 2, 2022

Evaluation Criteria



Upcoming Funding Announcements

June/July
- Carbon Storage Validation & Testing
- Rare Earth Elements Demonstration Facility
- Rare Earth Mineral Security
- Solar Energy RD&D

July/August
- Enhanced Geothermal Systems Demos
- Direct Air Capture Hubs
- Preventing Outages and Enhancing the Resilience of the Electric Grid State Grants ▲
- Hydropower RD&D
- State Energy Program ▲
- Energy Efficient Transformer Rebate Program
- Extended Product Systems Rebate Program
- EE and Renewable Improvement at Public School Facilities
- Carbon Capture Technology Program, Front-End Engineering and Design

August/September
- Regional Clean Hydrogen Hubs
- Clean Hydrogen Manufacturing Recycling RD&D Program
- Clean Hydrogen Electrolysis Program
- Energy Storage Demonstration Projects
- Long Duration Demonstration Initiative
- Energy Improvement in Rural and Remote Areas
- Critical Material Innovation, Efficiency and Alternatives
- Marine Energy RD&D

And more to come in Fall 2022!

To receive updates on all funding announcements subscribe at: Energy.gov/BIL

▲ Formula awards, all others competitive solicitations

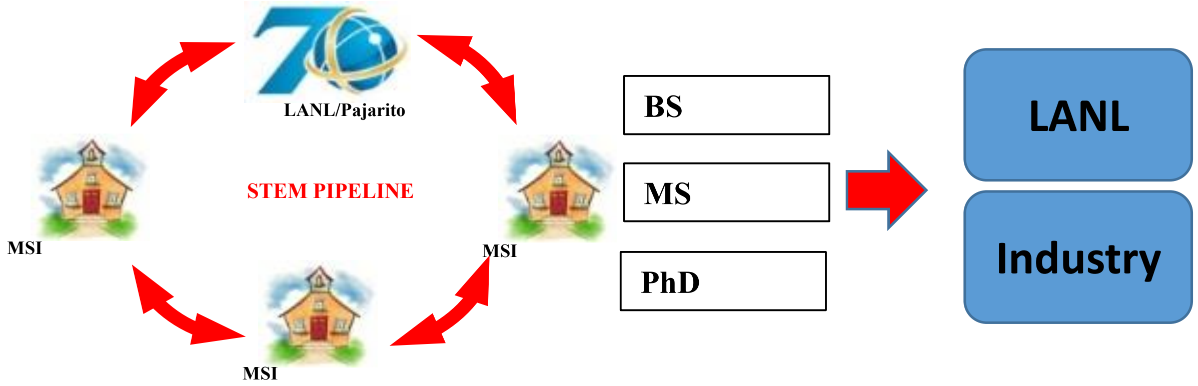
Promoting Diversity, Equity & Inclusion:

Pajarito Powder & LANL hosts Industry day
Discuss research opportunities plus facility tour
Building an alliance for MSI industry internships

HFTO/MSIPP/LANL/Pajarito Powder Establishes Collaboration with MSIs

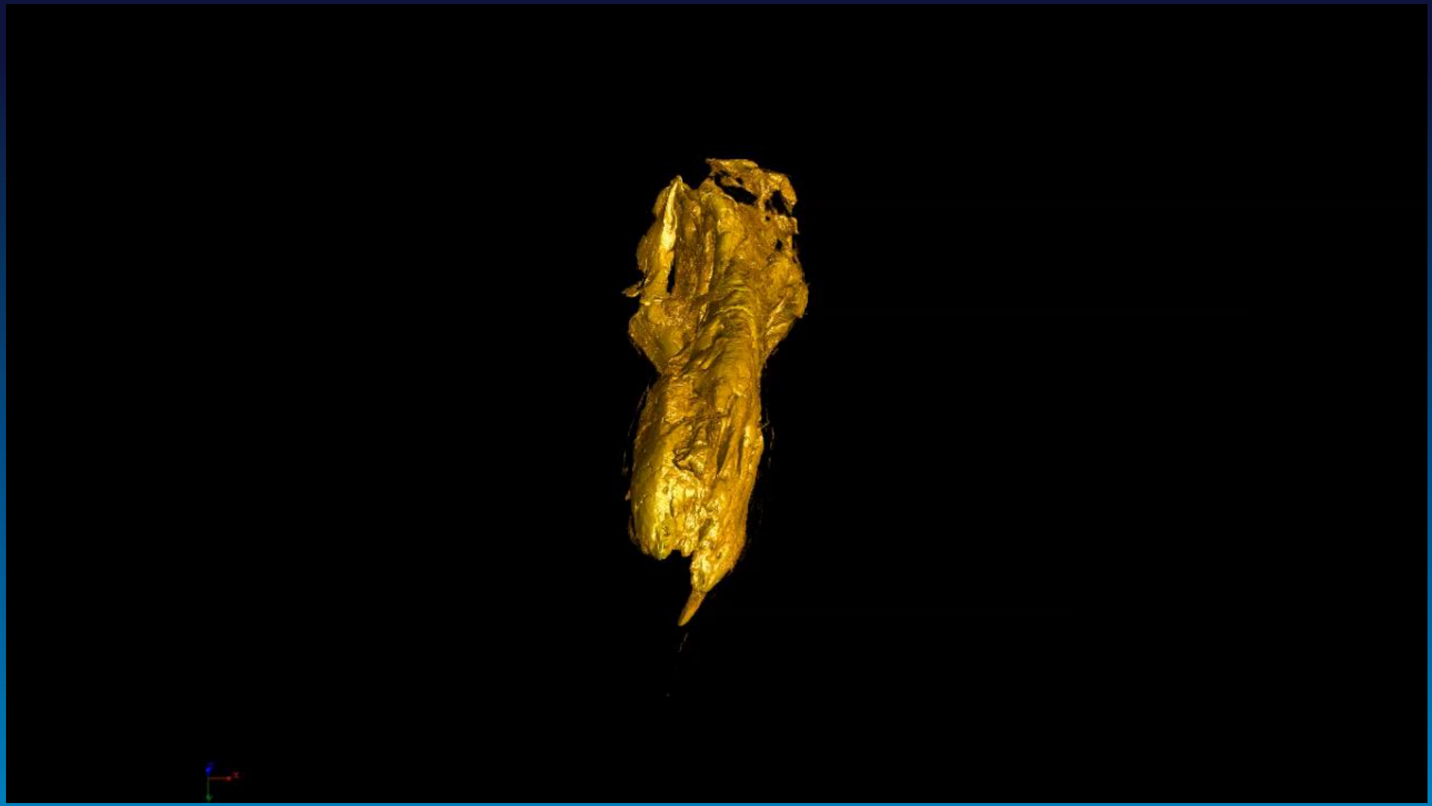
Project Goals:

- Develop a mutually beneficial relationship between HFTO, LANL, Industry Partners, and MSIs
- Promote MSI involvement with Fuel Cell and Electrolysis-related research
- Provide opportunities for MSI scholars to perform cutting-edge FC research at LANL
- Encourage MSI scholars to pursue advanced degrees and enter the Hydrogen and Fuel Cell Workforce



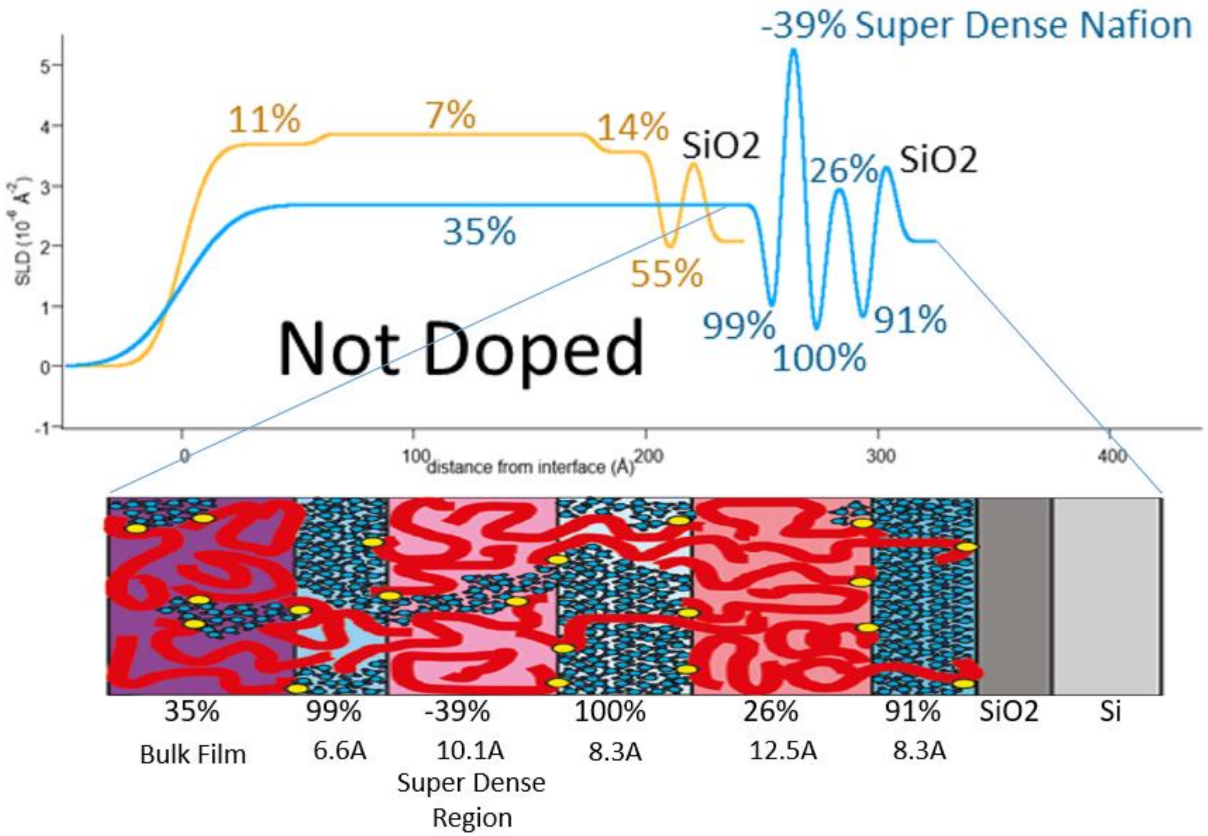
E-6: NON-DESTRUCTIVE TESTING & EVALUATION

- Inspection Methods
  - Ultrasonic Testing (UT)
  - Eddy Current Testing (ET)
  - Radiography (RT, CT)
  - Penetrant Testing (PT)
  - Magnetic Particle Testing (MPT)
  - X-ray Fluorescence (XRF)
  - Visual Inspection (VT)
  - Nuclear Magnetic Resonance (NMR)
- ~50 X-ray Generators (10keV-20MeV)
- CT and DR Imaging Detectors (100um pixel)
- UT- TOF, Phased UT systems, Traditional systems
- XRF, Thermography, LIBs
- Traditional and Phased Eddy Current Systems
- Magnetic Particle Bench and Portable Systems
- Various Penetrant Methods

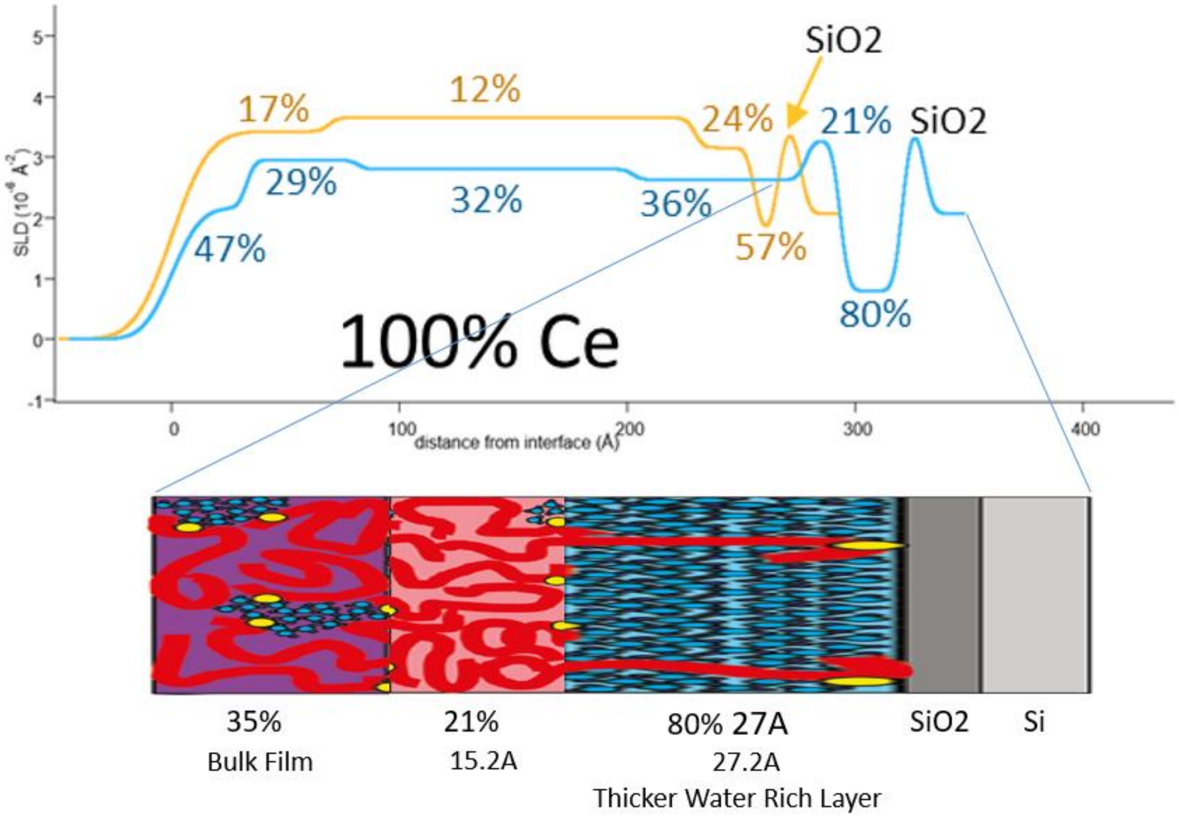


Effect of Cations (Ce, Co) on Nafion Interfacial Structure

Undoped Nafion Film Structure (Hydrated)

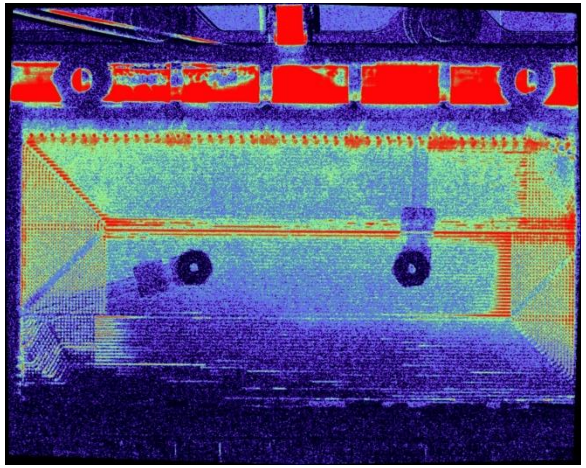


Doped Nafion Film Structure (Hydrated)

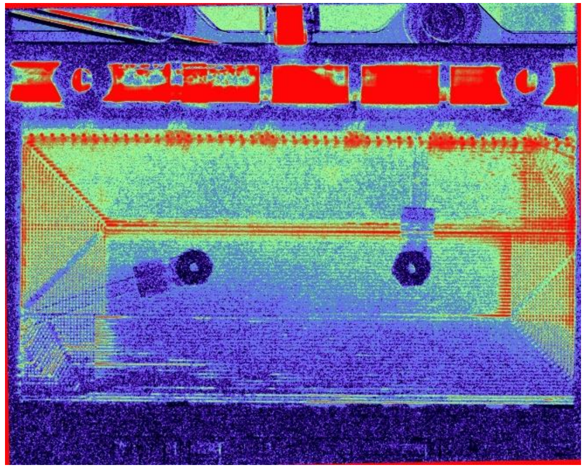


Short-Stack of Toyota Mirai Fuel Cell Matrix

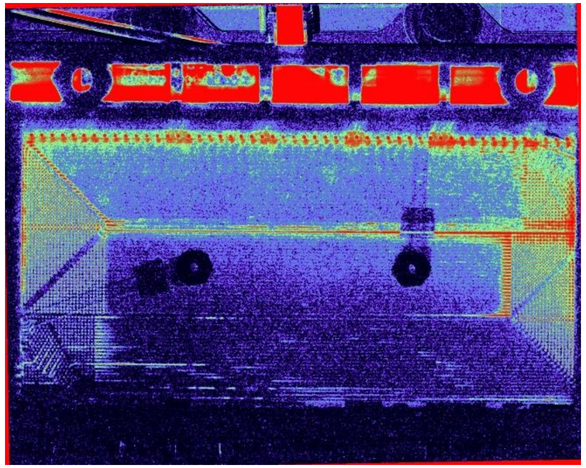
50A



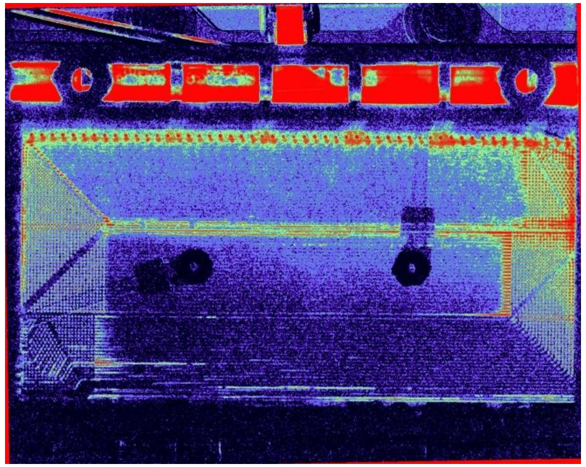
70A



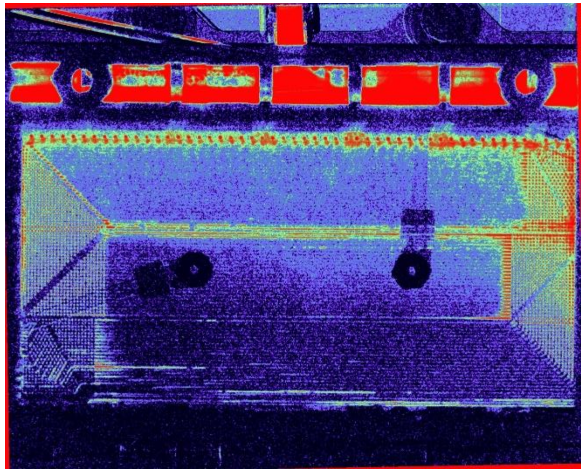
87.5A



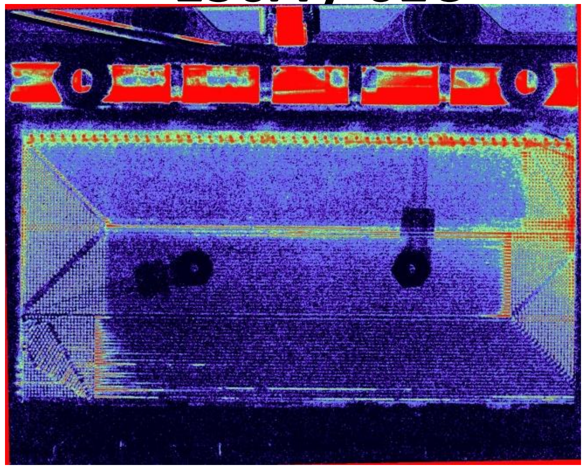
105A



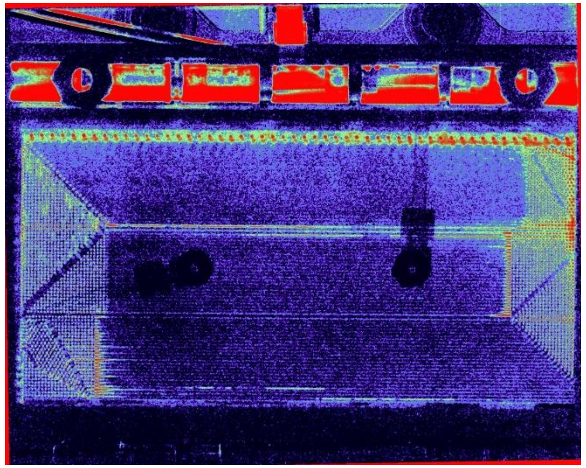
125A



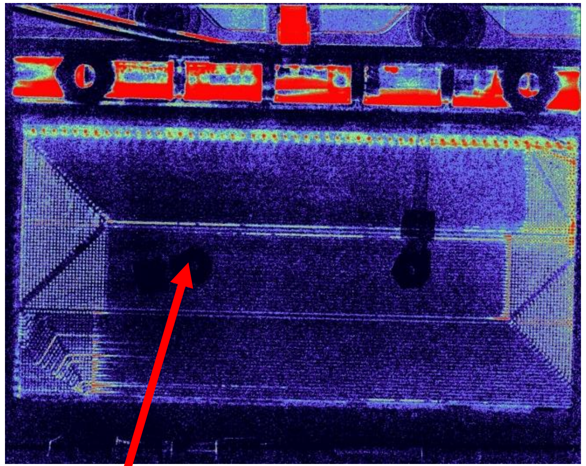
150A / 61C



225A



312A



High Current & Flowrates show much less liquid water than low current/flowrates

Notes: ***12.5 Amp point, unstable***

450 Amp point insufficient H2

FCPAD
FUEL CELL PERFORMANCE AND DURABILITY

Our national security mission is broad and important
— and is motivated and enabled by ST&E discovery

Ensure the safety, reliability, and performance of the U.S nuclear stockpile

- Physics & Design
- Engineering & Weaponization
- Production

Excellence in nuclear security
to ensure the nation's nuclear deterrent through theory, modeling and simulation, and experimentation

Preventing and countering
efforts of proliferants to acquire, develop or disseminate materials and expertise necessary for nuclear weapons

Energy security

- Sustainable Clean Energy
- Resilient Materials
- Complexity in Energy Systems

Capability Pillars define six key areas of science, technology, and engineering in which we must innovate and excel.

The Pillars steer institutional investments, which are then leveraged by DOE programs.

Materials for the Future	Defects and Interfaces Extreme Environments Emergent Phenomena
Nuclear and Particle Futures	Applied Nuclear Science & Engineering Nuclear & Particle Physics, Astrophysics & Cosmology Accelerator Science & Technology High Energy Density Physics & Fluid Dynamics
Integrating Information, Science, and Technology for Prediction	Computing Platforms Computational Methods Data Science
Science of Signatures	Natural and Anthropogenic Phenomena Nuclear Detonation Nuclear Processing, Movement, Weaponization
Complex Natural and Engineered Systems	Human–Natural System Interactions Engineered Systems
Weapons Systems	Design Manufacturing Analysis

Energy security challenges are prioritized in R&D investments across most Capability Pillars

MATERIALS FOR THE FUTURE

SCIENCE OF SIGNATURES

COMPLEX NATURAL AND ENGINEERED SYSTEMS

INTEGRATING IS&T FOR PREDICTION

NUCLEAR AND PARTICLE FUTURES

WEAPONS SYSTEMS

Materials for the Future

Fuel Cells
Polymer Electrolyte Membrane (PEM) technology

Materials and process development: PGM-free catalysts, alkaline membranes, and enhancing durability of fuel cell components

Critical Materials
- Selective extraction of REEs from low-temp geothermal fluids
- Co-mingling desalination with the production of critical materials
- Hybrid methods for supercritical desalination

Science of Signatures

Signals from Noise
Using machine learning to extract more knowledge from geophysical signals from geothermal systems and other subsurface environments

Complex Natural and Engineered Systems

Advanced Algae Systems
Algae as a bio-feedstock for fuels and bioproducts

Feedstock and Logistics
Addressing woody biomass and corn stover processing bottlenecks

Biomass Conversion
Technologies for conversion into biofuels, bioproducts, and biopower synthesis

Advanced Development and Optimization
Integrating individual technologies into a system/process

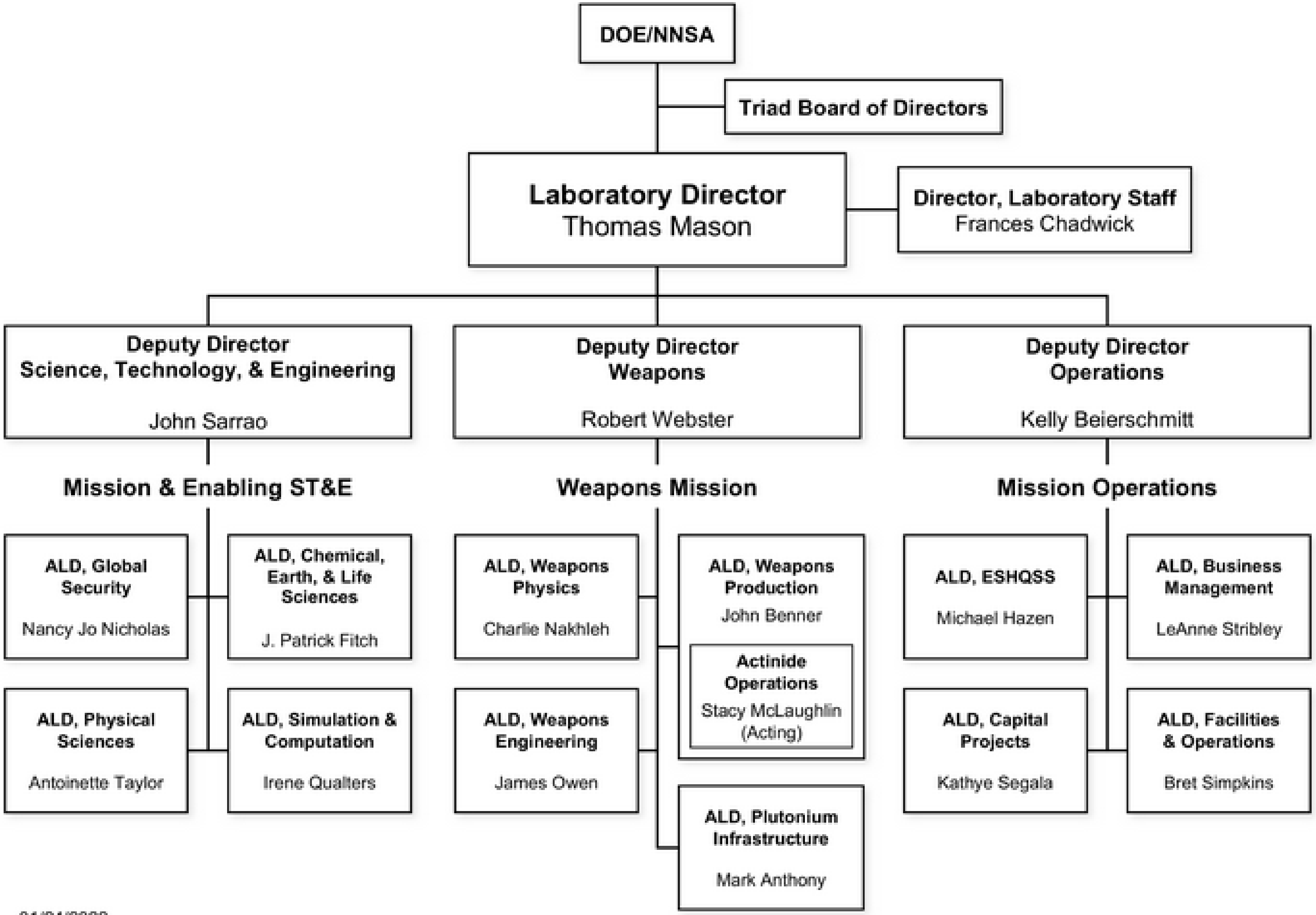
Integrating IS&T for Prediction

Advanced Grid Modeling
- Integrated control and optimization under uncertainty
- Interdependent energy networks
- Design of resilient power systems
- Analysis of extreme events and threats

Cyber Security for Energy Delivery Systems
Algorithms for optimal grid design to minimize the impact of cyber-physical attacks on the power grid

Infrastructure Security and Energy Restoration
Data analytics and modeling to deliver a catalog of historical weather-related outage events

Los Alamos National Laboratory



01/24/2022

Physical Sciences Directorate

Associate Laboratory Director
Antoinette (Toni) Taylor

LANSCE User Facility
Mike Furlanetto

- **Accelerator Strategy Office**
  Juan Barraza
- **LANSCE Facility Operations**
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  Charles Kelsey, DFOD

Chief Operating Officer
Raeanna Sharp-Geiger

Staff Operations Manager
Liana Lovato
Office Administrators:
Christina Villareal
Regina Martinez

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Mark Gulley, DDL

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- **National High Magnetic Field Laboratory Group (MPA-MAG)** – Ross McDonald (Acting)
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- **Nuclear & Particle Physics & Applications Group (P-3)** – Melynda Brooks
- **Thermonuclear Plasma Physics Group (P-4)** – Dmitry Yarotski

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- **Finishing Manufacturing Science Group (Sigma-2)** – Jennifer McEahern
- **Sigma Operations Group (Sigma-Ops)** – Tanner Trujillo

Physical Sciences Program Office

Office of Science Programs
Srinivas Iyer

Civilian Nuclear Program Office
DV Rao

BIL Hydrogen Provisions cover Range of RDD&D

Manufacturing RD&D across H_2 and fuel cell technologies

Raw Materials → **Processed Materials** → **Subcomponents** → **End Product**

Includes end of life (EOL) & recycling RD&D

Sec. 40314 (EPACT Sec 815): Clean Hydrogen Manufacturing & Recycling **$0.5 Billion over 5 years**

Electrolysis RD&D: BIL Includes RD&D across multiple electrolysis technologies, compression, storage, drying, integrated systems, etc.

Sec. 40314 (EPACT Sec 816): Clean Hydrogen Electrolysis Program; **$1 Billion over 5 years. Goal $2/kg by 2026**

Regional Clean H_2 Hubs: At least 4 Hubs, geographic diversity, includes renewables, fossil + CCS, nuclear, for clean hydrogen production, multiple end use applications

Sec. 40314 (EPACT Sec 813): Regional Clean Hydrogen Hubs; **$8 Billion over 5 years**

National Hydrogen Strategy and Roadmap: Within 180 days

Clean Hydrogen Standard: 2 kg CO_2e/kg H_2, update within 5 yrs

Sec. 40314 (EPACT Sec 814: Strategy & Roadmap and **Sec. 40315 (EPACT Sec 822)**: Clean Hydrogen Production Qualifications)

Scope And Process

Example Stakeholders

H_2 Producers & Source

- Renewables
- Fossil Fuels (+CCS)
- Nuclear

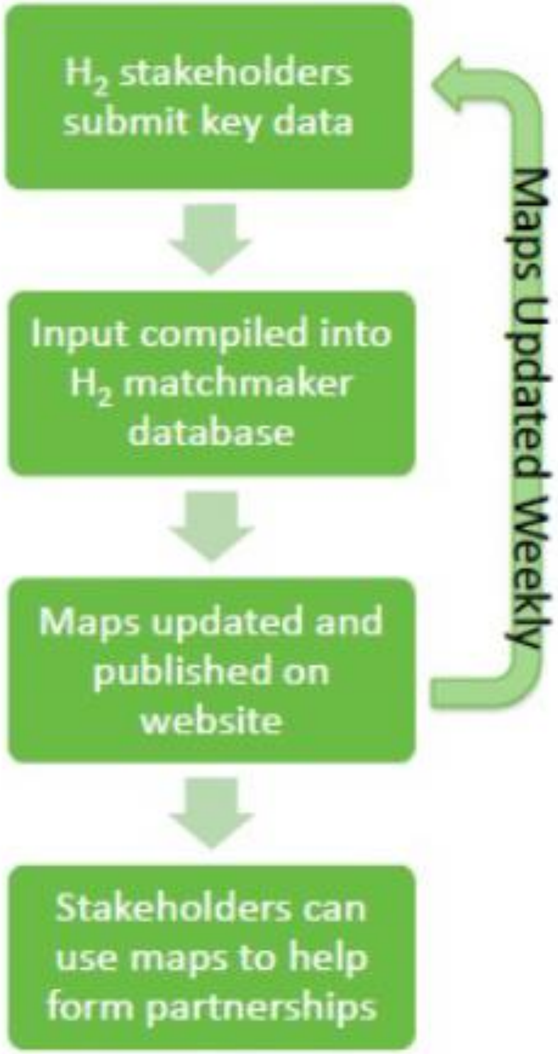
H_2 Consumers

- Electrical power production
- Industrial use
- Residential and commercial heating
- Transportation

H_2 Infrastructure Operators

- H_2 bulk storage
- H_2 compatible pipelines
- Fueling Stations
- H_2 delivery solutions

Matchmaker Process



Membrane AST development

Chemours visit

May 24th 2022

LANL Durability, FC-PAD and M2FCT Teams

Los Alamos

Current ASTs

Chemical : H_2/Air : 90 ^oC 30%RH

Table P.3 MEA Chemical Stability and Metrics (Test Using an MEA)		
Test condition	Steady-state OCV, single cell 25–50 cm^2	
Total time	500 h	
Temperature	90°C	
Relative humidity	Anode/cathode 30/30%	
Fuel/oxidant	H_2/air at stoics of 10/10 at 0.2 A/cm^2 equivalent flow	
Pressure, outlet kPa abs	Anode/cathode 150/150	
Metric	**Frequency**	**Target**
F^- release or equivalent for nonfluorinated membranes	At least every 24 h	No target—for monitoring
Hydrogen crossover (mA/cm^2) [a, b]	Every 24 h	≤15 mA/cm^2
OCV [b, c]	Continuous	Initial OCV ≥ 0.95 V, <20% OCV decrease during test
High-frequency resistance	Every 24 h at 0.2 A/cm^2	No target—for monitoring
Shorting resistance [d]	Every 24 h	>1,000 ohm cm^2

[a] Tested in MEA on H_2, 80°C, fully humidified gases, 1 atm total pressure. See M. Inaba et. al., *Electrochimica Acta*, 51 (2006): 5746.
[b] Hydrogen crossover and OCV targets should be achieved at 0 kPa pressure differential and at 50 kPa anode overpressure relative to cathode, providing sensitivity to global membrane thinning and to hole formation, respectively.
[c] A protocol such as the one shown in Table P.9 should be used to recover reversible losses at least once every 24 h and prior to measuring each metric.
[d] Measured at 0.5 V applied potential, 80°C, 100% RH N_2/N_2. Compression to 20% strain on the GDL.

Mechanical : Air/Air 80 ^oC wet/dry

Table P.4 Membrane Mechanical Cycle and Metrics (Test Using an MEA)		
Cycle	Cycle 0% RH (2 min) to 90°C dew point (2 min), single cell 25-50 cm^2	
Total time	Until crossover >15 mA/cm^2 or 20,000 cycles	
Temperature	80°C	
Relative humidity	Cycle from 0% RH (2 min) to 90°C dew point (2 min)	
Fuel/oxidant	Air/air at 2 SLPM on both sides	
Pressure	Ambient or no back pressure	
Metric	**Frequency**	**Target**
Crossover [a]	Every 24 h	≤15 mA/cm^2 [b]
Shorting resistance [c]	Every 24 h	>1,000 ohm cm^2

[a] Tested in MEA on H_2, 80°C, fully humidified gases, 1 atm total pressure. See M. Inaba et. al., *Electrochimica Acta*, 51 (2006): 5746. Crossover recorded after 2 min of drying under 0% RH conditions. Hydrogen crossover target should be achieved at 0 kPa pressure differential and at 50 kPa anode overpressure, providing sensitivity to global membrane thinning and to hole formation, respectively.
[b] For air or N_2 testing, an equivalent crossover metric of 0.1 sccm/cm^2 at a 20 kPa pressure differential, 80°C, and 100%RH may be used as an alternative.
[c] Measured at 0.5 V applied potential, 80°C and 100% RH N_2/N_2. Compression to 20% strain on the GDL.

Current ASTs

Combined : H_2/Air : 90 ^oC wet (30s)/Dry(45s)

Table P.5 Membrane Chemical/Mechanical Cycle and Metrics (Test Using an MEA)		
Cycle	Cycle 0% RH (30 s) to 90°C dew point (45 s), single cell 25-50 cm^2	
Total time	Until crossover >15 mA/cm^2 or 20,000 cycles	
Temperature	90°C	
Relative humidity	Cycle from 0% RH (30 s) to 90°C dew point (45 s) [a]	
Fuel/oxidant	H_2/air at 40 $sccm/cm^2$ on both sides	
Pressure	Ambient or no back pressure	
Metric	**Frequency**	**Target**
F- release or equivalent for Nonfluorine membranes	At least every 24 h	No target—for monitoring
Hydrogen crossover (mA/cm^2) [b, c]	Every 24 h	<15 mA/cm^2
OCV [c, d]	Continuous	Initial wet OCV ≥ 0.95 V, <20% OCV decrease during test
High-frequency resistance	Every 24 h at 0.2 A/cm^2	No target—for monitoring
Shorting resistance [e]	Every 24 h	>1,000 ohm cm^2

[a] Step durations of 30 s dry and 45 s wet were selected in testing at LANL so that the HFR at the end of the dry step was 2.5 times the HFR at the end of the wet step, which is approximately equal to the HFR ratio that occurs when running the mechanical test (Table P.4). Depending on the hardware used, these step times may need to be adjusted to achieve the same HFR variation.

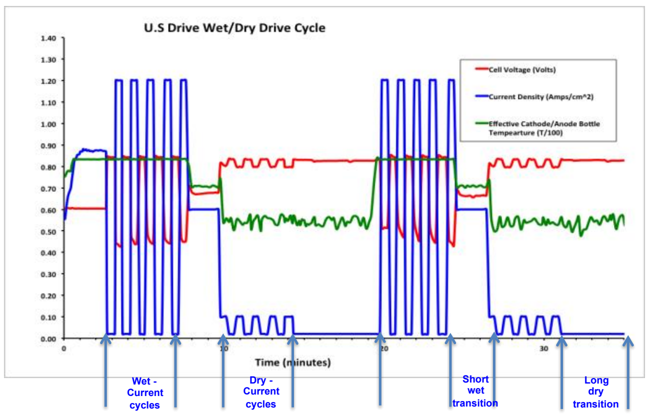
[b] Tested in MEA on H_2, 80°C, fully humidified gases, 1 atm total pressure. See M. Inaba, et. al., *Electrochimica Acta*, 51 (2006): 5746. Crossover recorded after 2 min of drying under 0% RH conditions.

[c] Hydrogen crossover and OCV targets should be achieved at 0 kPa pressure differential and at 50 kPa anode overpressure, providing sensitivity to global membrane thinning and to hole formation, respectively.

[d] A protocol such as the one shown in Table P.9 should be used to recover reversible losses at least once every 24 h and prior to measuring each metric.

[e] Measured at 0.5 V applied potential, 80°C, 100% RH N_2/N_2. Compression to 20% strain on the GDL.

Durability Testing Protocol



Target = 5000 hours

Durability protocol

Wet : T_{cell}=85 ^oC, T_{Sat}=83 ^oC

0.02 to 1.2A/cm^2 (2 s each)

Dry : T_{cell}=80 ^oC, T_{Sat}=53 ^oC

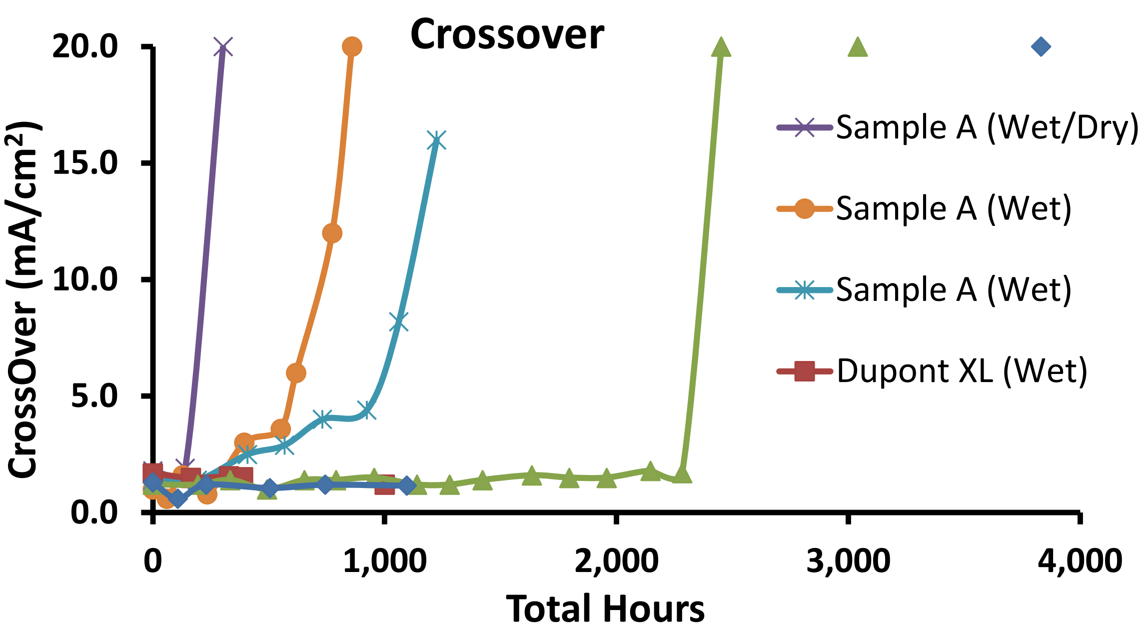
0.02 to 0.1A/cm^2 (2 s each)

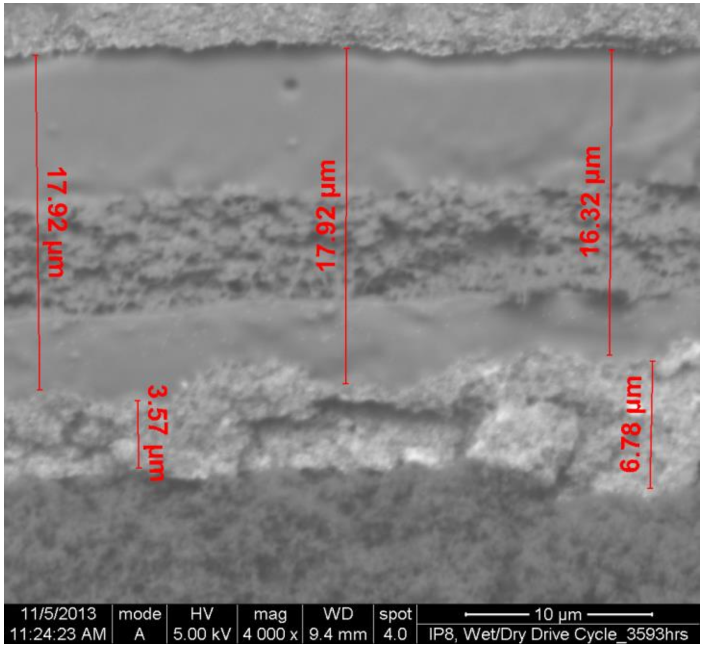
Table P.7 Drive-Cycle Durability Protocol [a, b, c]

Test Point #	Current Density (A/cm^2)	Anode H_2 Stoich.	Anode Dew Point Temp. (°C)	Anode Inlet Temp. (°C)	Cathode O_2 Stoich.	Cathode Dew Point Temp. (°C)	Cathode Inlet Temp. (°C)	Test Point Run Time (min)	Worst-Case Response Transition Time (s)
Wet with Load Cycling									
RH1	0.02	96	83°	85°	108	83°	85°	0.5	2
RH2	1.2	1.6	83°	85°	1.8	83°	85°	0.5	2
RH3	0.02	96	83°	85°	108	83°	85°	0.5	2
RH4	1.2	1.6	83°	85°	1.8	83°	85°	0.5	2
RH5	0.02	96	83°	85°	108	83°	85°	0.5	2
RH6	1.2	1.6	83°	85°	1.8	83°	85°	0.5	2
RH7	0.02	96	83°	85°	108	83°	85°	0.5	2
RH8	1.2	1.6	83°	85°	1.8	83°	85°	0.5	2
RH9	0.02	96	83°	85°	108	83°	85°	0.5	2
RH10	1.2	1.6	83°	85°	1.8	83°	85°	0.5	2
Trans1	0.6	2	70°	80°	2	70°	80°	2	30 (dew point)
Dry with Load Cycling									
RH11	0.1	5	53°	80°	5	53°	80°	0.5	30 (dew point)
RH12	0.02	25	53°	80°	25	53°	80°	0.5	2
RH13	0.1	5	53°	80°	5	53°	80°	0.5	2
RH14	0.02	25	53°	80°	25	53°	80°	0.5	2
RH15	0.1	5	53°	80°	5	53°	80°	0.5	2
RH16	0.02	25	53°	80°	25	53°	80°	0.5	2
RH17	0.1	5	53°	80°	5	53°	80°	0.5	2
RH18	0.02	25	53°	80°	25	53°	80°	0.5	2

Membrane Degradation : FCTT Drive Cycle

Membrane AST



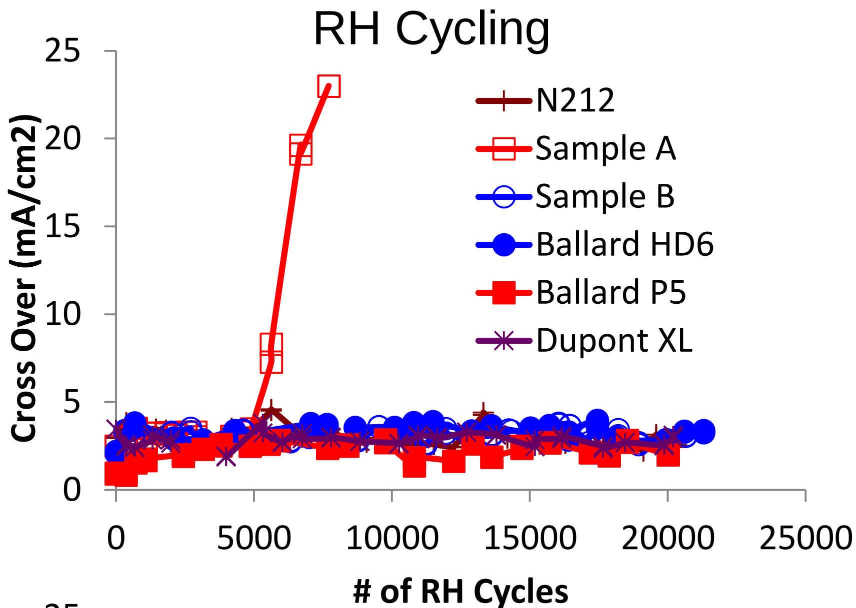


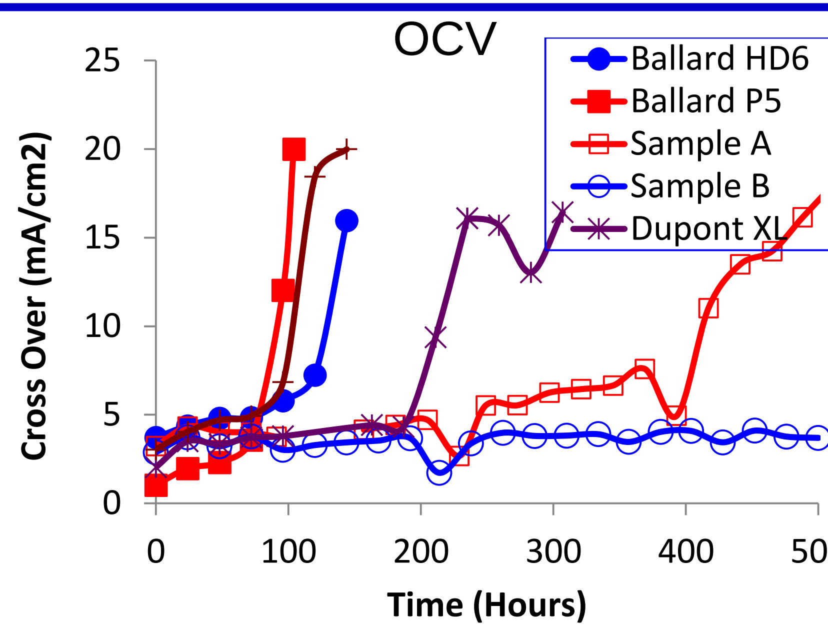
- Membranes without chemical and mechanical stabilization fail early in the drive cycle tests (< 500 hours) and fail even under wet only testing (< 1000 hours)
- Membranes with chemical and mechanical stabilization (DuPont XL®) last > 2500 hours
  - ✓ One sample failed at 2300 hours due to test stand failure
  - ✓ The DuPont XL® membrane failed at the edges due to absence of sub gasket
    - ✓ After 3800 hours: ≈ 30% thinning (mainly on cathode side of support)

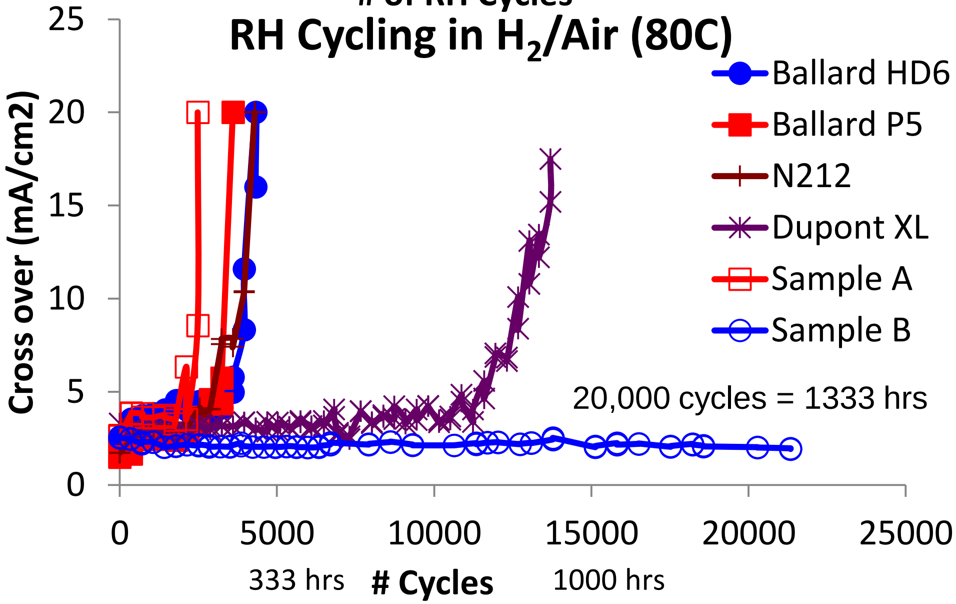
Journal of The Electrochemical Society, 165 (6) F3085-F3093 (2018)

Los Alamos

Membrane Degradation : ASTs







- RH cycling test does not have ability to distinguish between most PFSA membranes
- OCV testing too severe compared to drive cycle where most membranes fail due to local tearing/thinning and due to global thinning
- Combined mechanical/chemical AST has ability to distinguish between MEAs, needs further acceleration.

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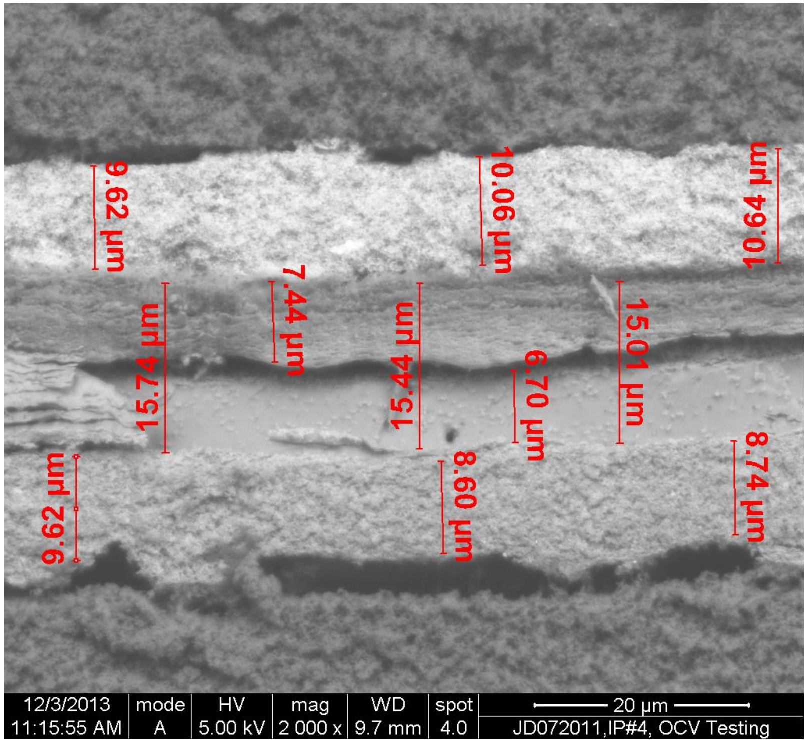
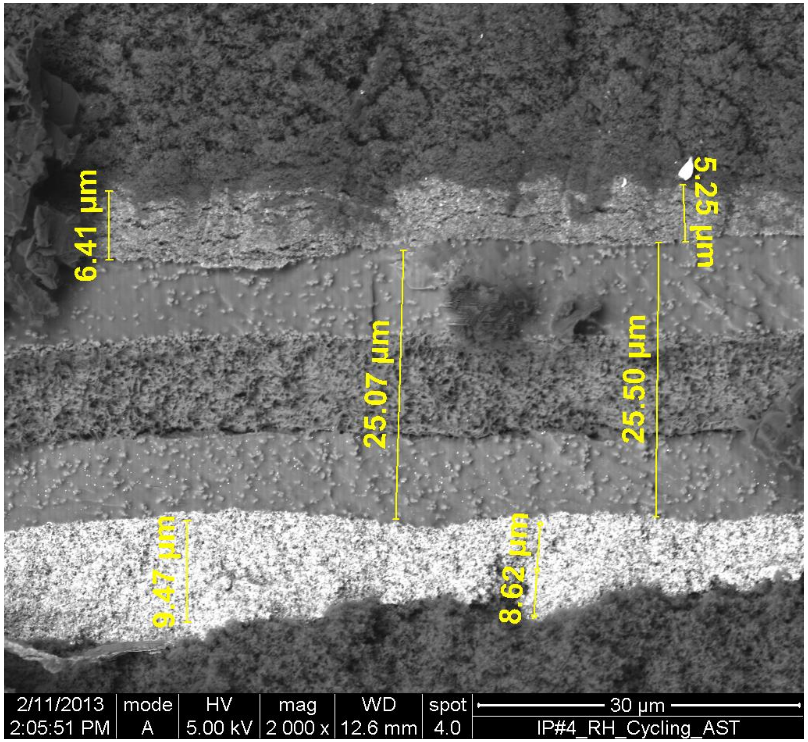
Membrane Degradation : ASTs

Membrane AST

DuPont XL® 307 hours @ OCV



DuPont XL® 20098 RH Cycles



- Chemical Degradation (OCV @ 90 ºC, 30% RH)
  - ✓ 40% membrane thinning observed after just 300+ hours of OCV testing
  - ✓ More severe compared to drive cycle and field data
- Mechanical Degradation (RH cycling @ 80 ºC in Air)
  - ✓ No visible degradation after 20,000 RH cycles
  - ✓ Most supported membranes are untouched by this AST

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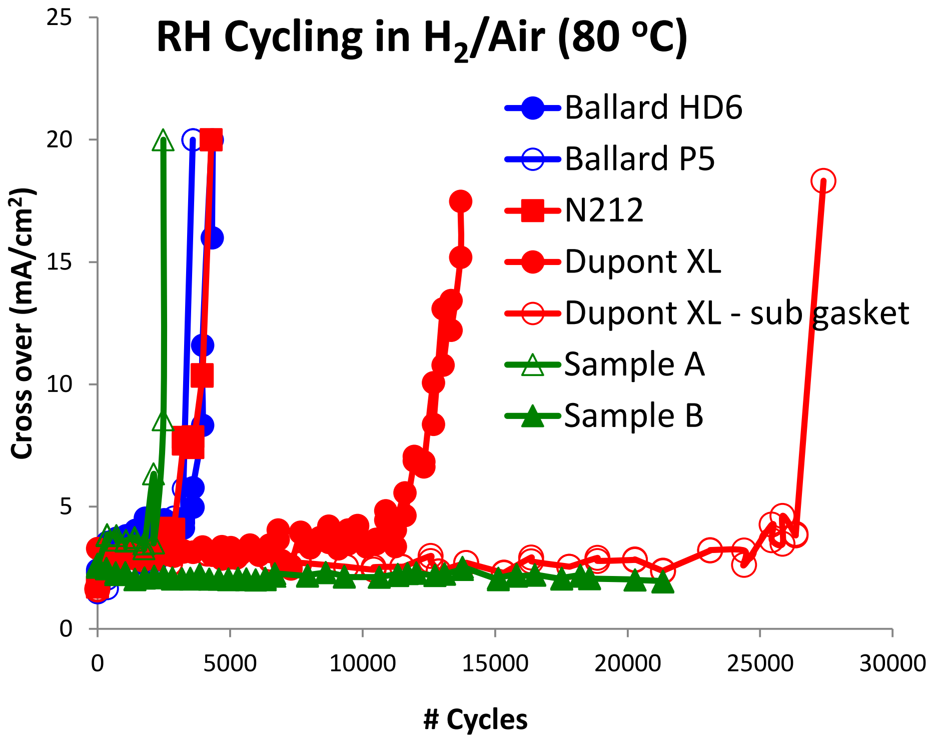
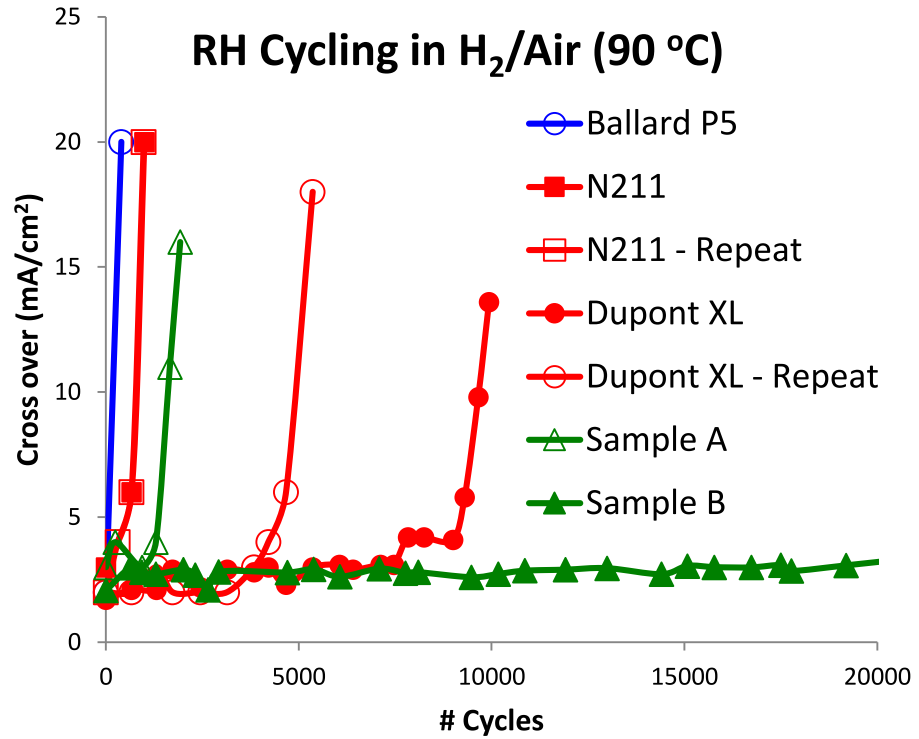
Membrane Degradation : ASTs

Membrane AST needing refinement

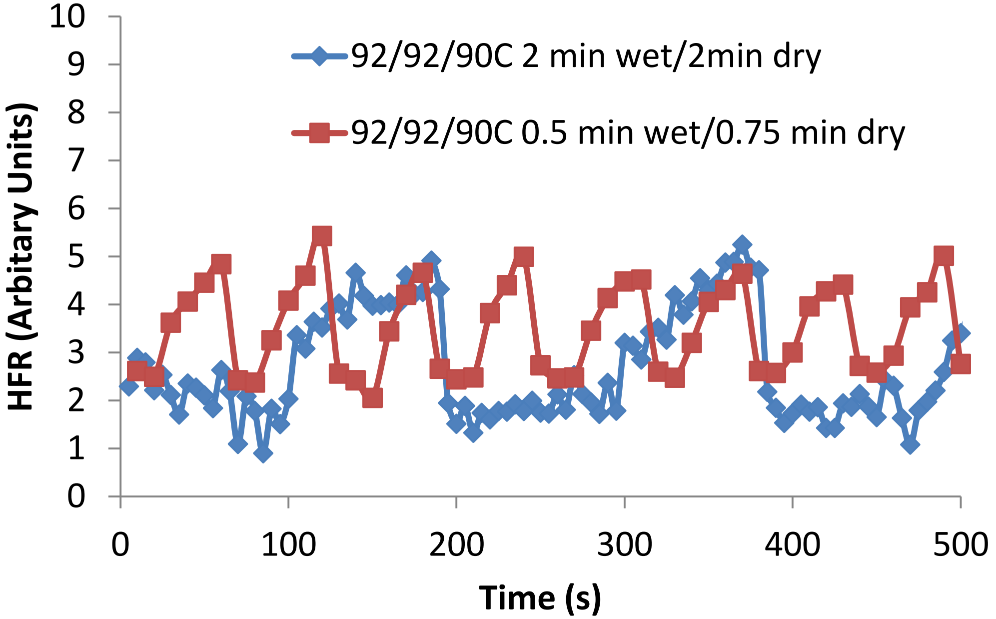


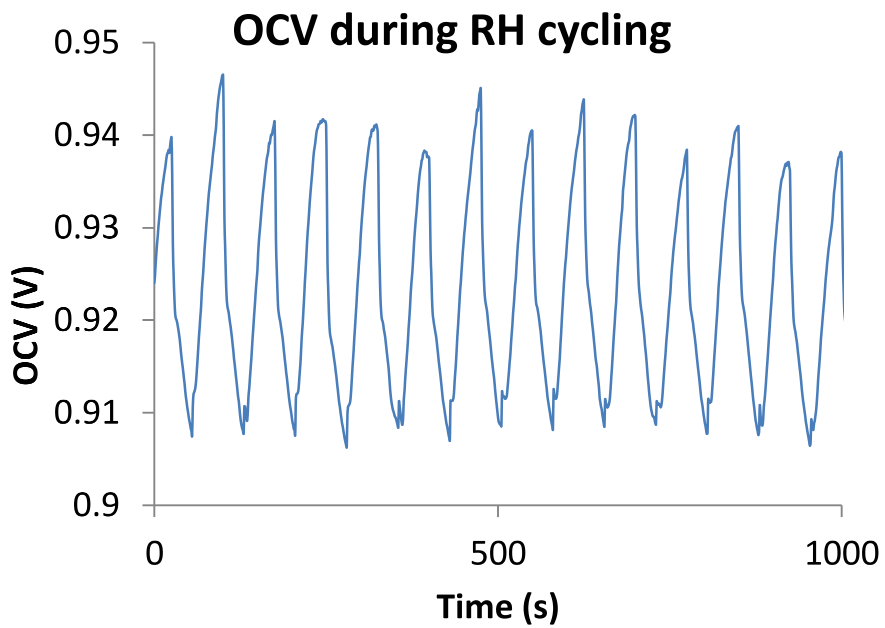


- RH cycling under OCV @ 80 ºC: Stabilized membranes last > 55 days (20,000 cycles)
- RH cycling under OCV @ 90 ºC: Thinning of N211 observed but still no thinning of DuPont XL®. Need to accelerate chemical degradation with respect to mechanical
- Increase time of dry cycle with respect to wet cycle keeping total cycle time constant

Current combined AST

- Uses 30sec wet and 45sec dry cycles: ≈ 3X faster cycling over 2min/2min
- Similar RH stresses as determined by HFR





- Un-stabilized sample fails at ≈ 1500 to 2000 cycles in this test which is similar to that in the 2min/2min cycling. A time acceleration of 3X. Time at OCV does not control failure but cycling does.
- Stabilized DuPont XL® fails in ≈ 25,000 to 30,000 cycles (625 hours) in this test and about ≈ 10,000 cycles (666 hours) in the previous test. Time at OCV is important not just # of cycles.

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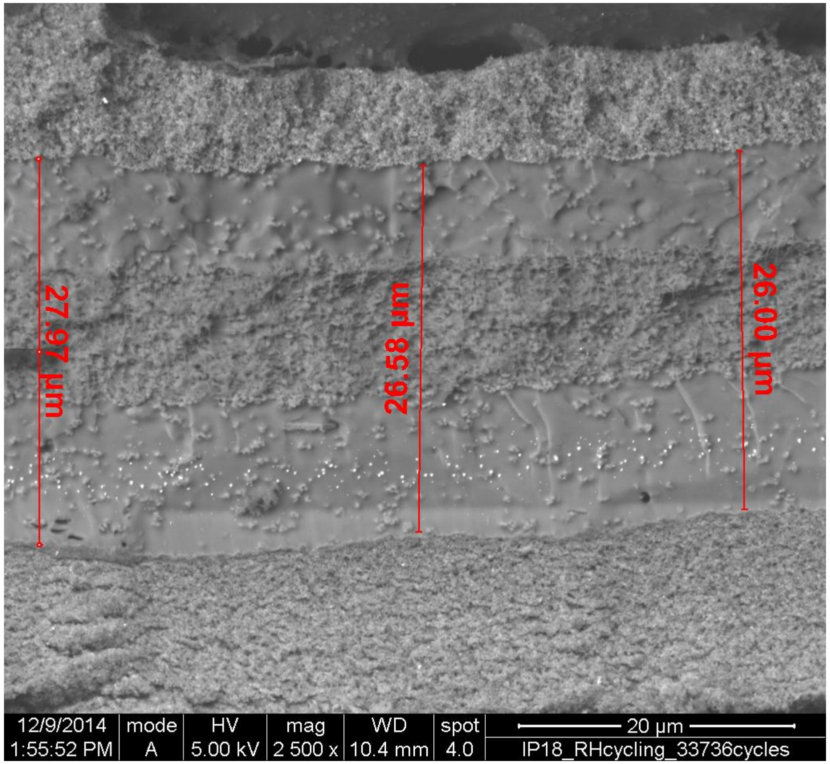
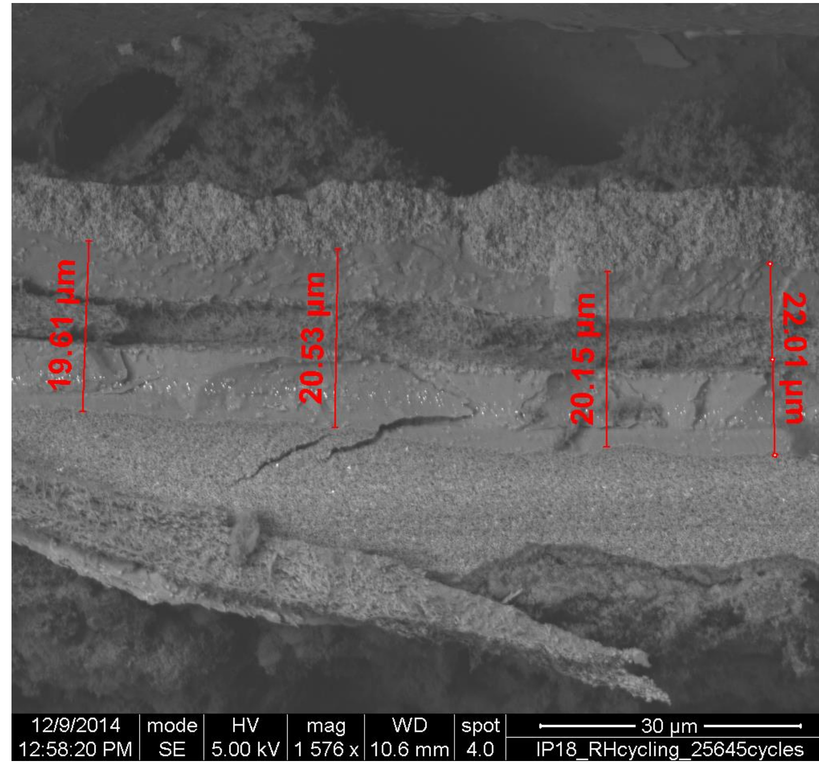
30sec/45sec RH cycling @ OCV

Middle



Edge



Clear evidence of Pt band on cathode side
Little global thinning observed

Current Understanding:
Sustainable Energy Fuels, 2017, 1, 409
Chem. Rev. 2017, 117, 987−1104

Clear evidence of Pt band on cathode side
Local thinning observed (from 25 µm to 20 µm): 20% thinning compared to 30% in drive cycle. More thinning on anode side
Cracking observed

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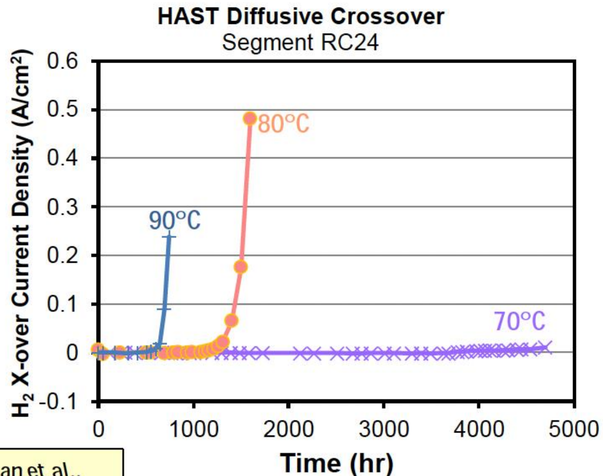
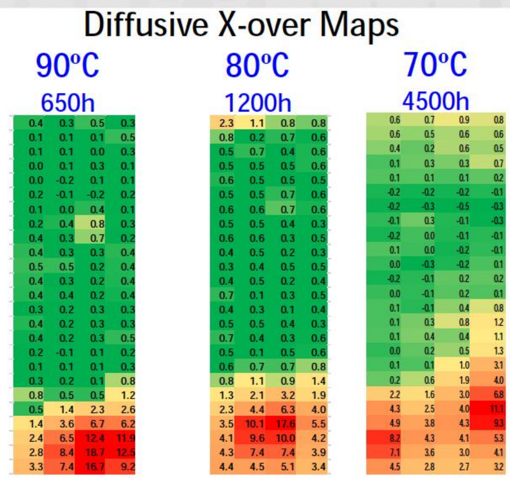
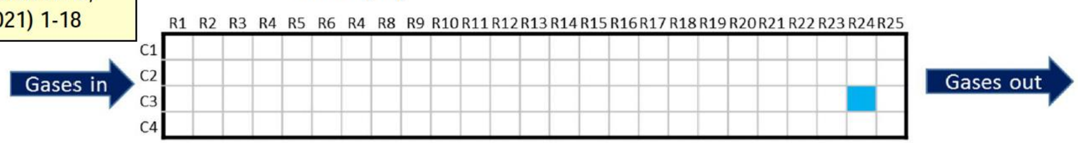
ASTWG and i-DWG

Impact of Temperature on Membrane Life





C. S. Gittleman et al., Joule, 5 (2021) 1-18



- Time to failure is strongly dependent on temperature
- Failure location (outlet) and failure mode (thinning) is similar at all temperatures.
- This has the required features of a good accelerated test: accelerated failure without changing the failure mode

- This MEA has run for over 10,000 hours (>14X acceleration factor) in a system level test using a 99% customer LDV duty cycle
- Suggests that 30,000h may be projected by about ~2000h of 90°C HALT

HYDROTEC GENERAL MOTORS | HYDROGEN FUEL CELL SOLUTIONS | ZERO EMISSIONS • MAXIMUM CAPABILITY

gm

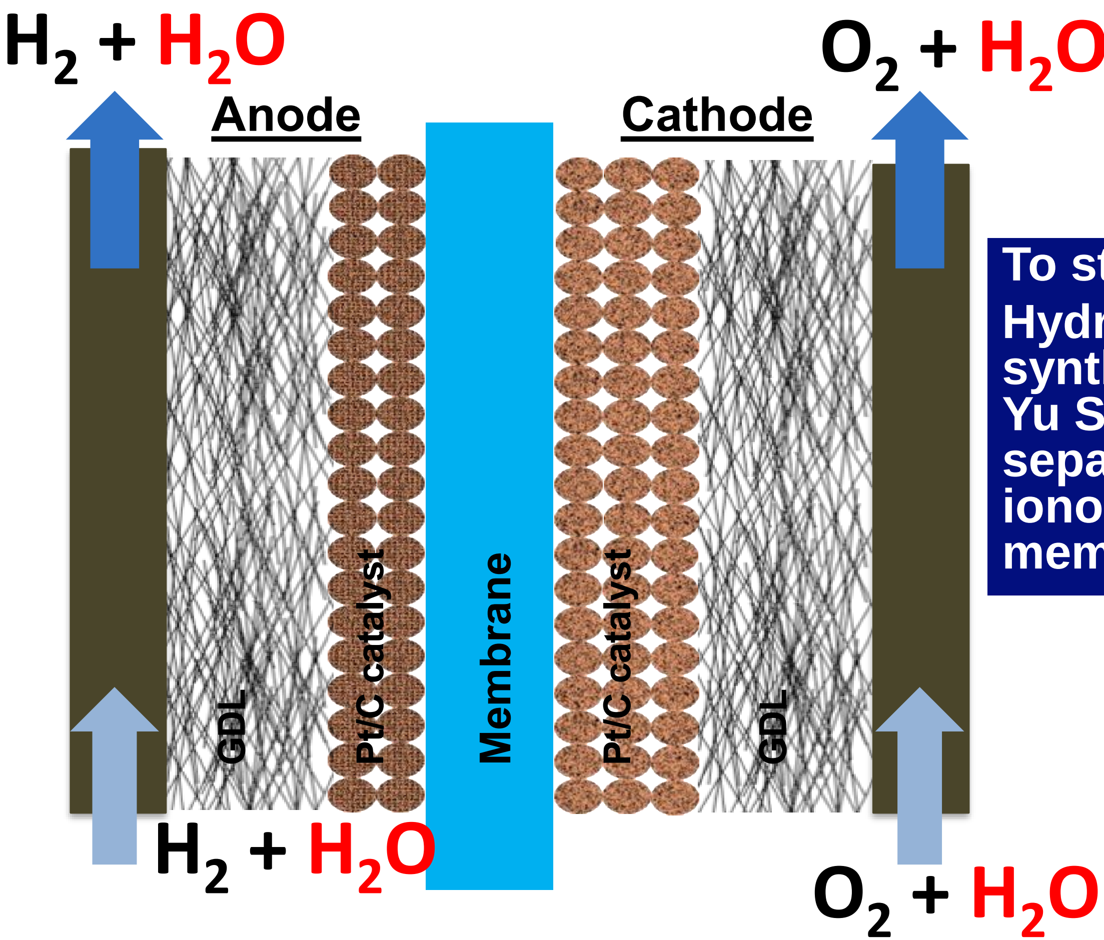
HAST -

Los Alamos

Heavy duty AST

- Currently using H_2/Air operation at 90 ^oC, 90%RH and potential cycling from 0.675V to 0.925V (30s each)
  - ≈ 55% ECSA loss and 65% MA loss after 500 hours
  - FER ≈ 3.5 $\mu g/cm^2$.hr for N211 and ≈ 1 $\mu g/cm^2$.hr for HP
- Will evaluate lower inlet RH to increase membrane degradation relative to catalyst degradation.

Ionomer Degradation



To study effect of HOPI in cathode:
Hydrocarbon membranes synthesized at LANL (Sarah park/ Yu Seung Kim) will be utilized to separate the degradation of ionomer in catalyst layer vs. membrane

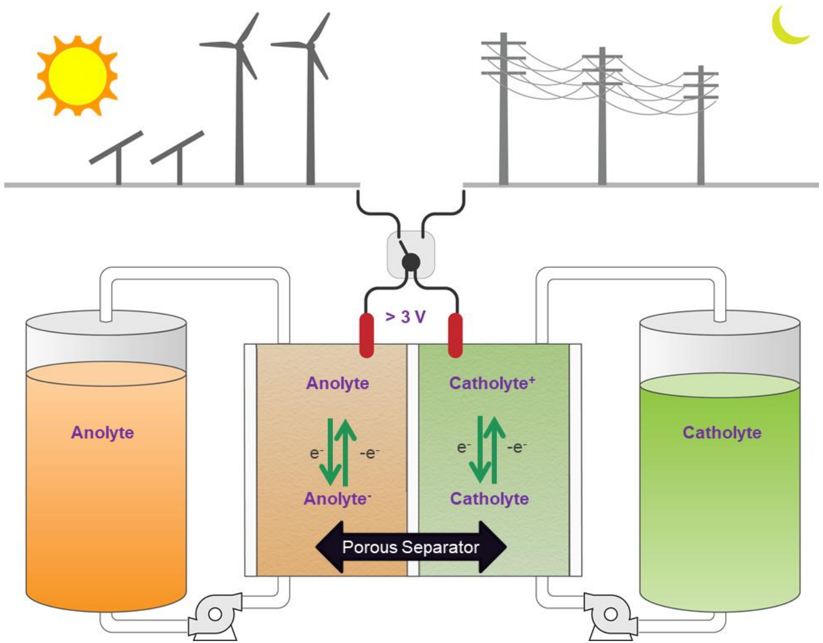
Redox Flow Batteries: Overview

Sandip Maurya

MPA-11: Materials physics and Applications Division

05/24/2022

LANL redox flow battery team



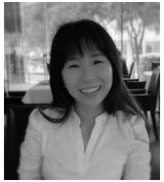
Flow battery development

Rangachary Mukundan, Sandip Maurya, Ben Davis



Membrane development

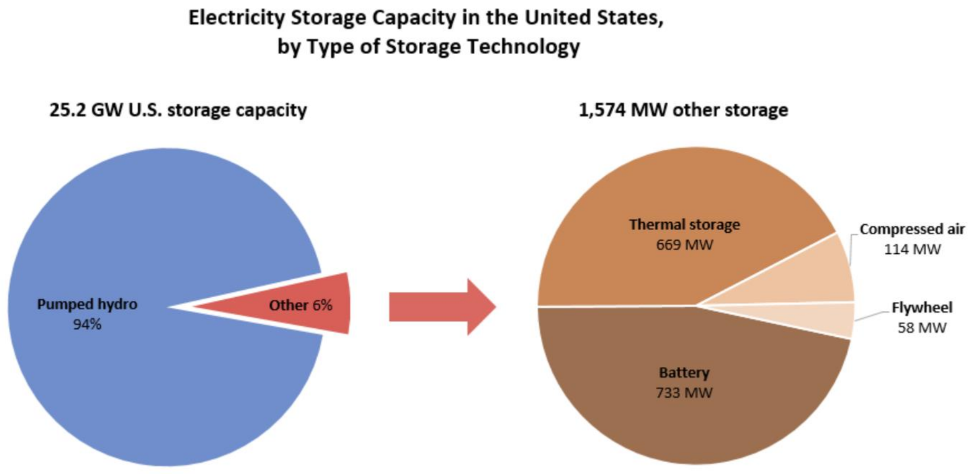
Sarah Park, Yu Seung Kim, Sandip Maurya



Members:

Thomas Stracensky
Kate Jesse
Sergio Diaz Abad
Travis Palmer
Gabe Andrade
Shikha Sharma
Carissa Yim

Electricity Storage in the United States



- Long duration energy storage(LDES) identified by the DOE as a key research area (one of three earth shots)
- DOE Office of Electricity has identified flow batteries as one of three core technologies for LDES

In 2050, ~1600 billion KWh electricity will be from intermittent renewable sources. Energy Storage in the US expected to grow 5-fold (125 – 400 GW). Most increase is battery storage

State of the art (Vanadium redox flow battery)

- more than 8 cycles/day
- 150-200% power overrating
- up to 94% efficiency
- > 25 years lifetime &
  > 15,000 cycles warranted
- highest safety standards:
  non-flammable
  non-explosive
- closed-loop recycling

Positive Electrode: $VO^{2+} + H_2O - e^- \rightarrow VO_2^+ + 2H^+$ (E^0 = 0.99 V vs. SHE)

Negative Electrode: $V^{3+} + e^- \rightarrow V^{2+}$ (E^0 = -0.26 V vs. SHE)

https://www.cellcube.com/

Commercially available VRFB systems
(> 30 companies, <u>Almost everyone use Nafion</u>)

Current DOE Targets (Near term and Long Term)

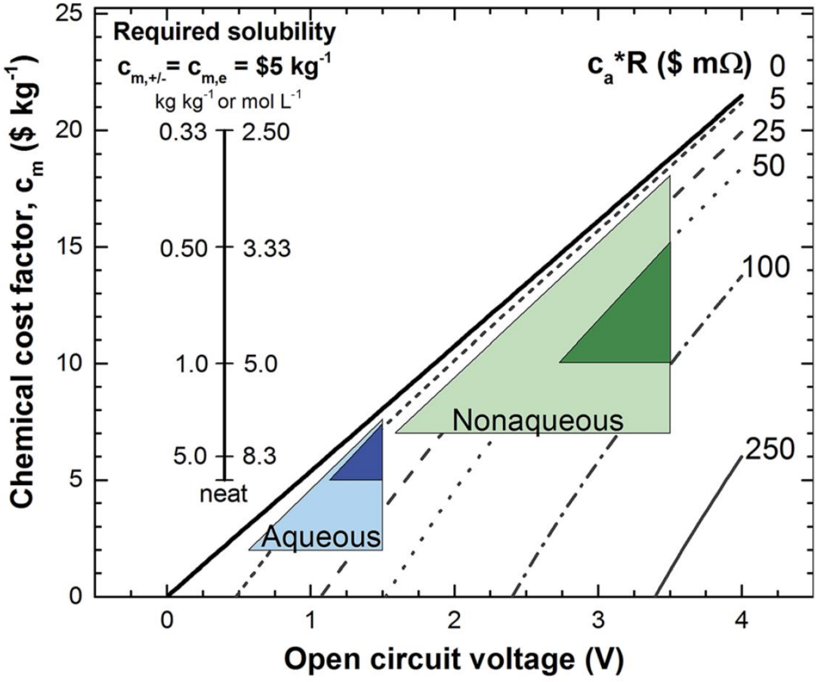
- Near: \$250 kWh^{-1} and LCOE = \$200 MWh^{-1}, 75% efficiency, 4000 cycles
- Long: \$150 kWh^{-1} and LCOE = \$100 MWh^{-1}, 80% efficiency, 5000 cycles

LCOE = Levelized cost of electricity

Low energy density

https://www.energy.gov/oe/activities/technology-development/energy-storage

Status of Non-Aqueous Redox Flow Battery



Robert Darling et al., Energy Envi. Sci. 7 (2014) 3459

- The DOE’s long term capital cost target:

  $100 – 150 per kWh
  ARPA-E: $100 per kWh
  OE: $150 per kWh

- According to cost modeling by JCESR and UTRC, the non-aqueous flow batteries have the potential to meet these cost targets.

- It is provided that the cost of active species are limited to $19/Kg and solubility is >2 M.

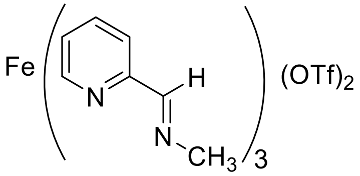
LANL capabilities for redox flow batteries

- Redox active molecule development
  - Iron Pyridylimine based metal-ligand coordinated compounds
    - Multi electron ligands and metal centers in symmetric configuration
  - Organic molecules
    - Symmetric and asymmetric configurations
- Membranes for flow battery systems
  - Quaternized poly(arylene ether benzonitrile) membranes developed for aqueous systems
  - Durable and Highly selective sulfonated Diels Alder Poly (phenylene) membranes for vanadium redox flow batteries
  - Determine transport number of the various species in aqueous and non-aqueous flow battery configurations

Synthesis and Electrochemical Characterizations
Theory/Prediction – Redox , Solubility and transport modeling

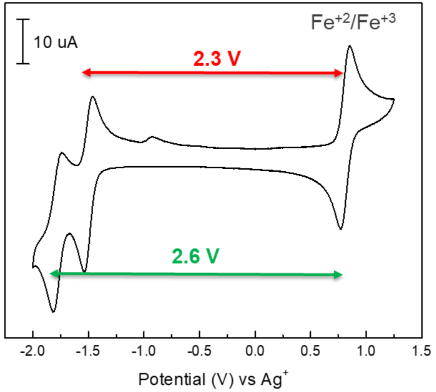
Redox active molecules development

Synthesis



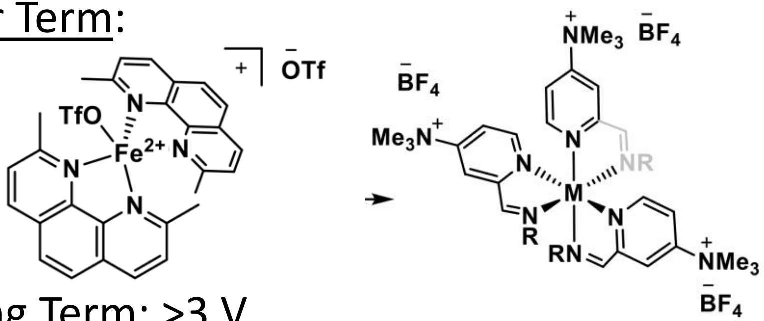
Fe(II) methylpyridylimine triflate

Cyclic Voltammetry

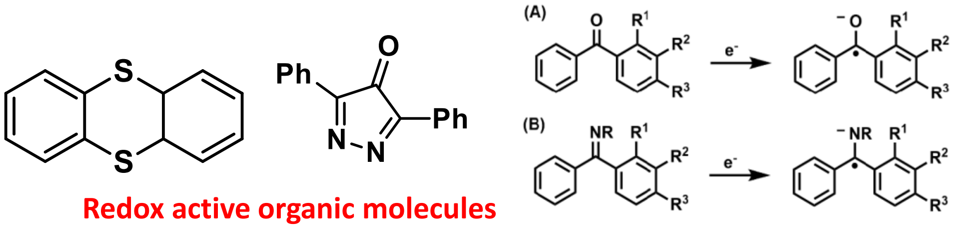


1 mM Fe(Me-PyIm) in 0.1 M $TBAPF_6$/ CH_3CN, 100 mV/s

Near Term:



Long Term: >3 V



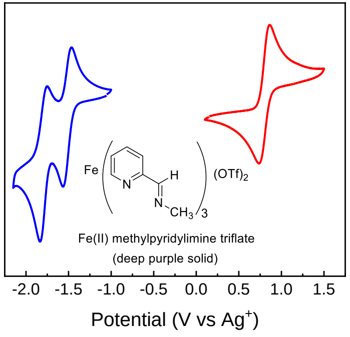
Redox active organic molecules

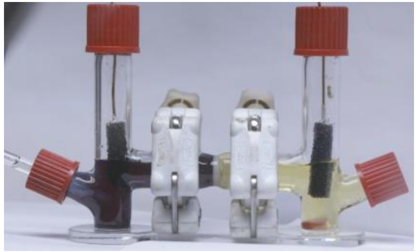
- Single charge species, redox separated by > 2V
- Upscaled for further cell testing
- Developing lower cost synthesis

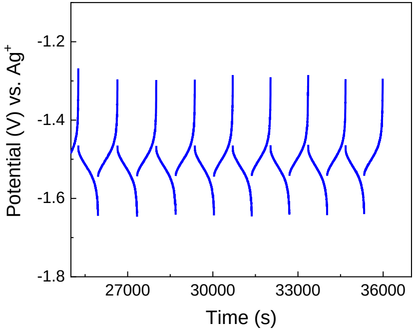
Sharma et al., Energy Storage Materials 37 (2021) 576-586
Chu et al., ChemsusChem 12 (2019) 1304-1309

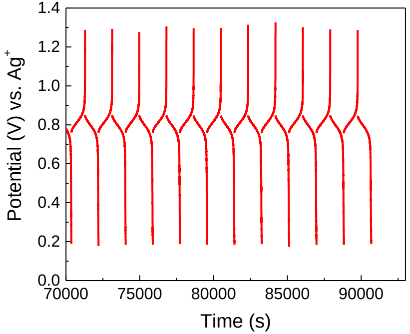
Electrochemical characterizations of redox couples

Bulk electrolysis

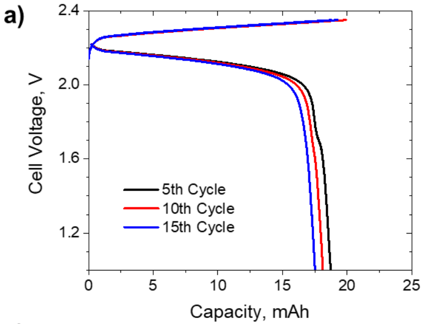


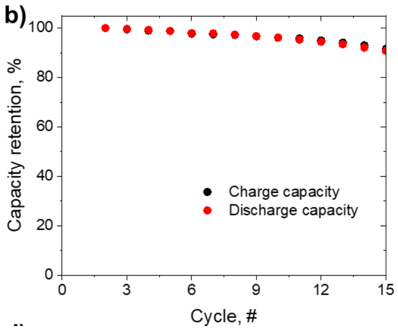


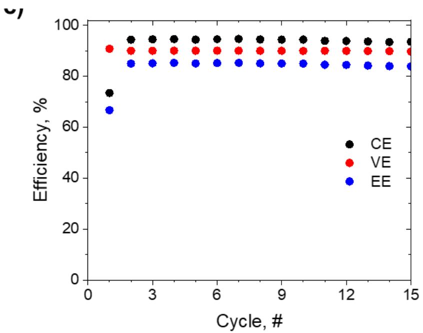


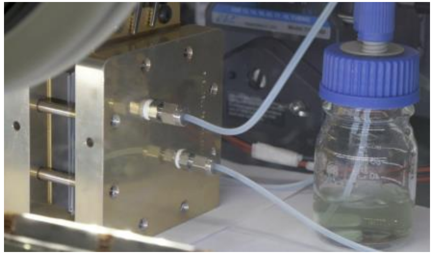


Flow battery cycling





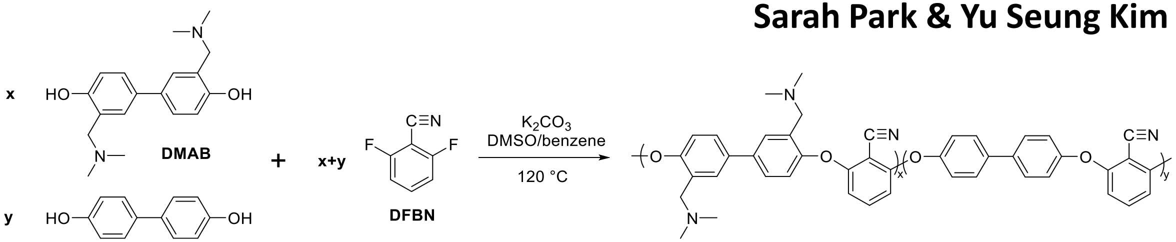


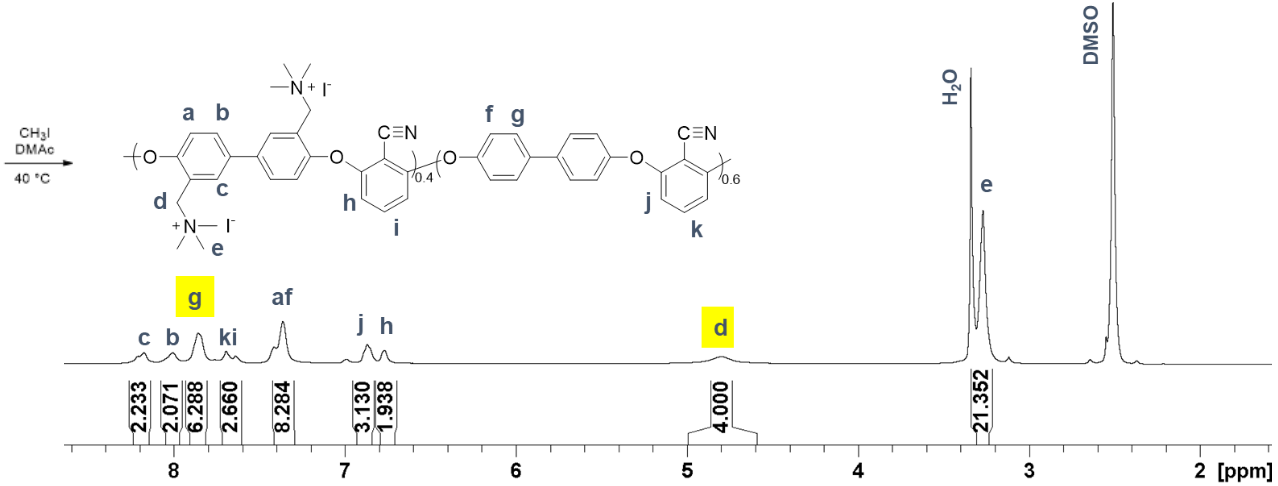


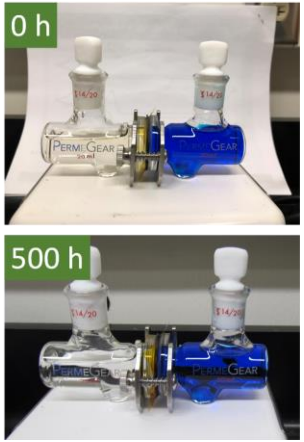
Sharma et al., Energy Storage Materials 37 (2021) 576-586

Membrane development

Sarah Park & Yu Seung Kim / MPA-11

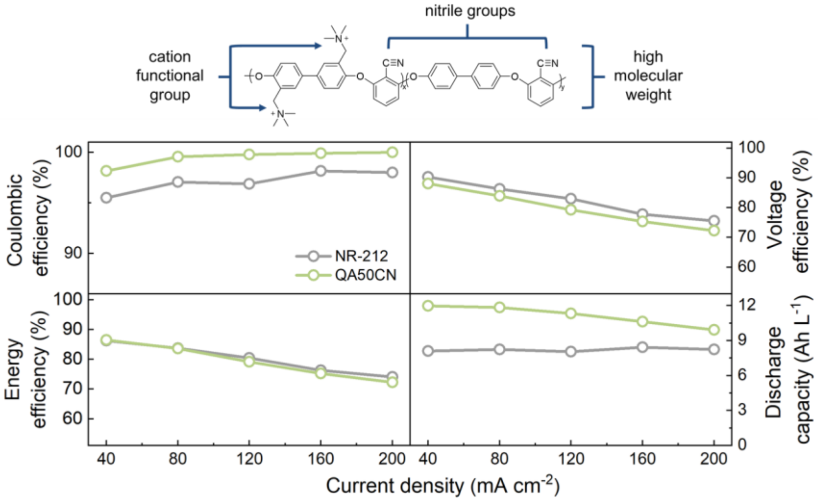


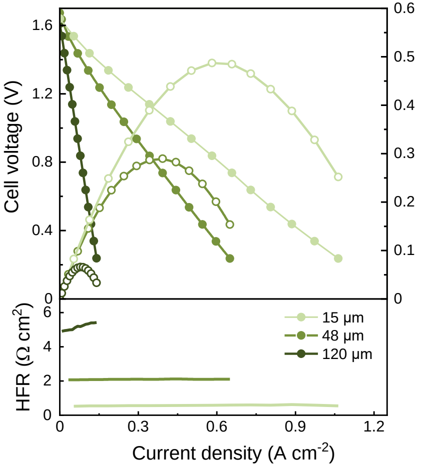


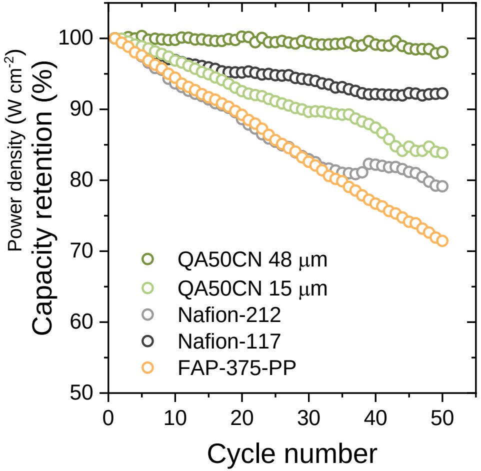


Park et al., Journal of Membrane Science 617 (2021) 118565

Membrane development







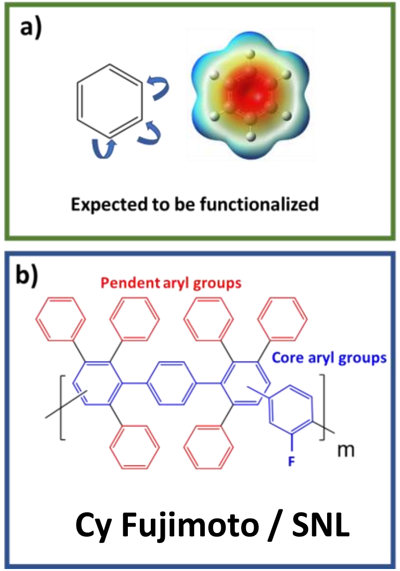
Quaternized poly(arylene ether benzonitrile) membranes: Synthesis and characterization

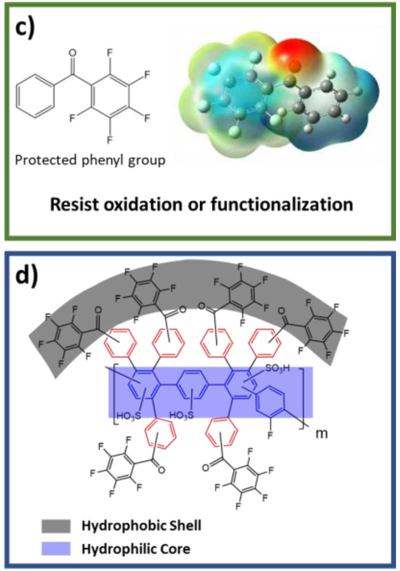
Performance comparable or better than SOA Nafion membrane in aqueous VRFB

- Stable anion exchange membranes developed
- Highly selective for Vanadium ions, No crossover in 500 h
- Performance optimization
- Decreased thickness : Improved power density; Increased thickness : Better capacity retention

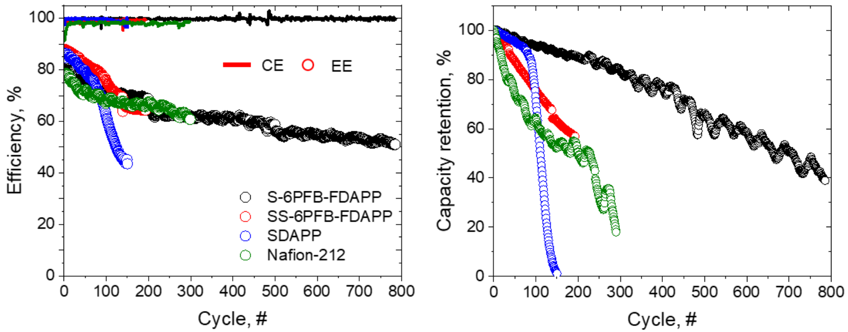
Park et al., Journal of Membrane Science 617 (2021) 118565

Membrane development





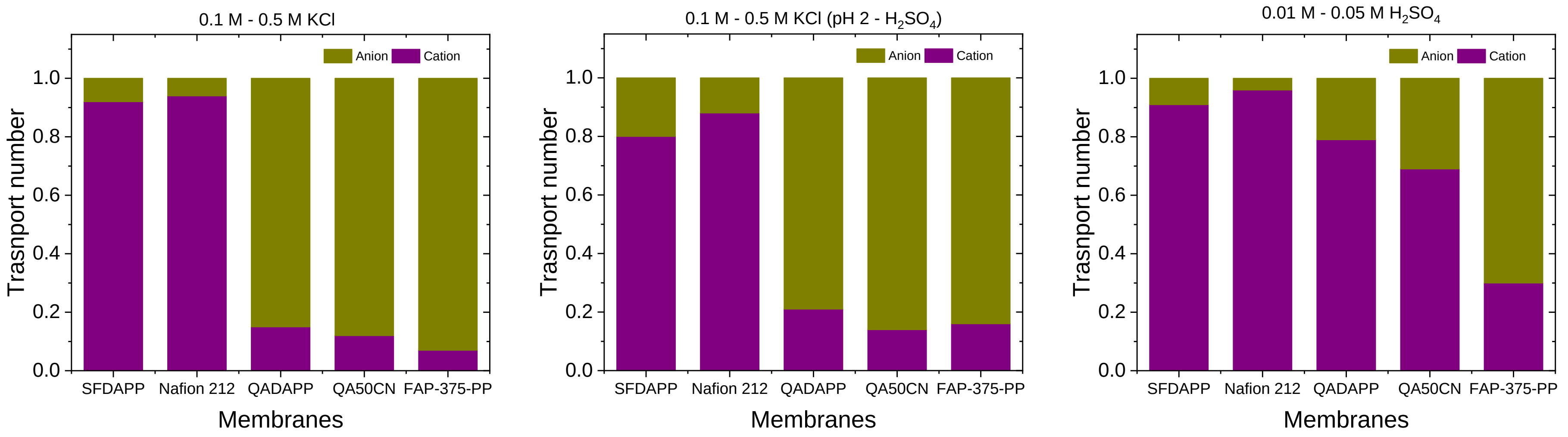
Membrane	IEC, meq g^{-1}	Uptake, %	Vanadium permeability, 10^{-7} cm^2 cm^{-1}	Proton Conductivity, mS cm^{-1}	Selectivity, 10^7 mS min cm^{-3}
S-6PFB-FDAPP	1.4	24	0.0425	4.3	10
SS-6PFB-FDAPP	1.8	36	8.15	8.7	1.1
Nafion-212	0.95	23	60	12.0	0.2



- Highly durable and selective sulfonated Diels Alder Poly(phenylene) based membranes were developed
- Better energy efficiencies (>99.9% CE) and comparable polarization performance.
- Extremely crossover minimizes the need of frequent rebalancing.

Maurya et al., Journal of Power Sources, 520 (2022) 230805

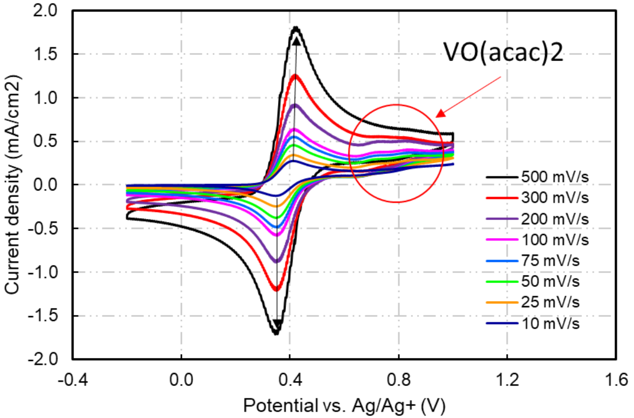
Identifying charge carriers in VRFBs

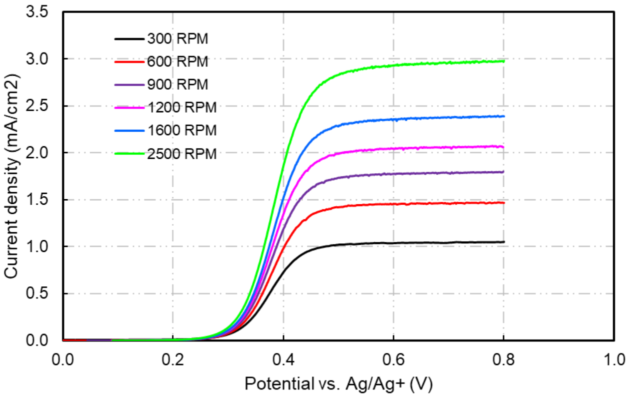


In collaboration with Cy Fujimoto @ SNL

- It is unclear what ions carry majority of charges in VRFB when AEM is employed.

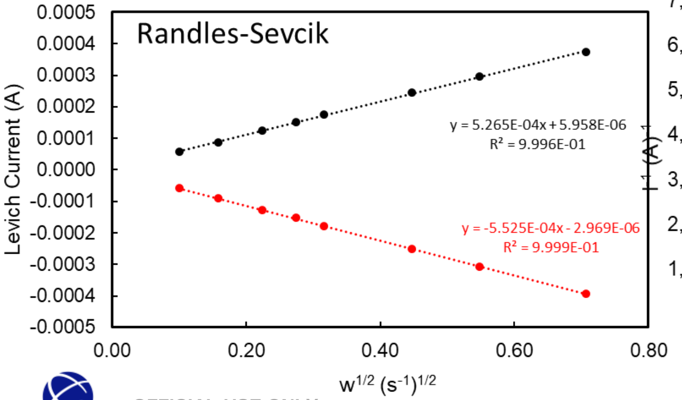
Electrochemical characterizations of redox couples

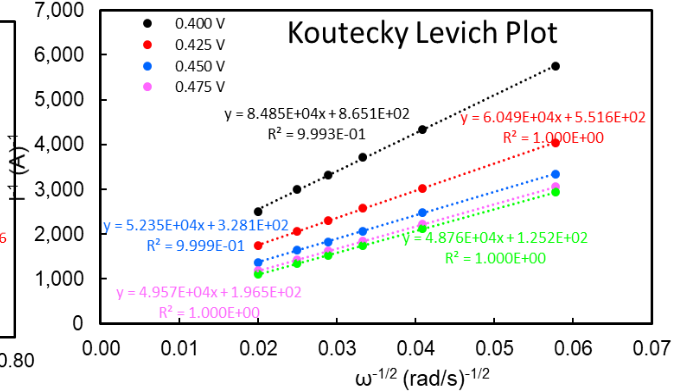


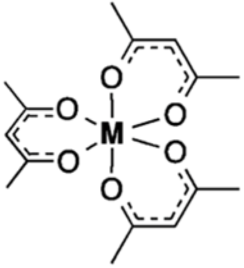


Fundamental electrochemistry

- Diffusion coefficients
- Kinetic currents
- Standard rate constant







M = V

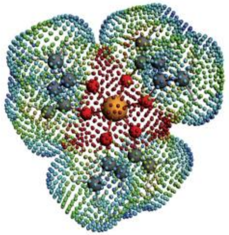
Other flow battery related capabilities

Solubility Modeling

Yang/Batista

RSC Advances 2019

PCCP Accepted 2019

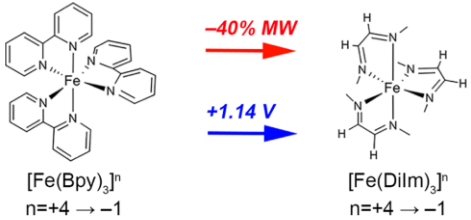


Redox Carrier Modelling

Yang/Batista

ACS Omega 2018

Frontiers in Physics, 2018



CFD modeling

Nguyen/Kang

Journal of power source, 2018

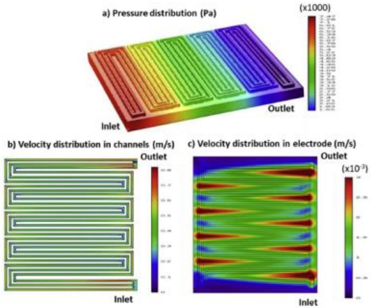
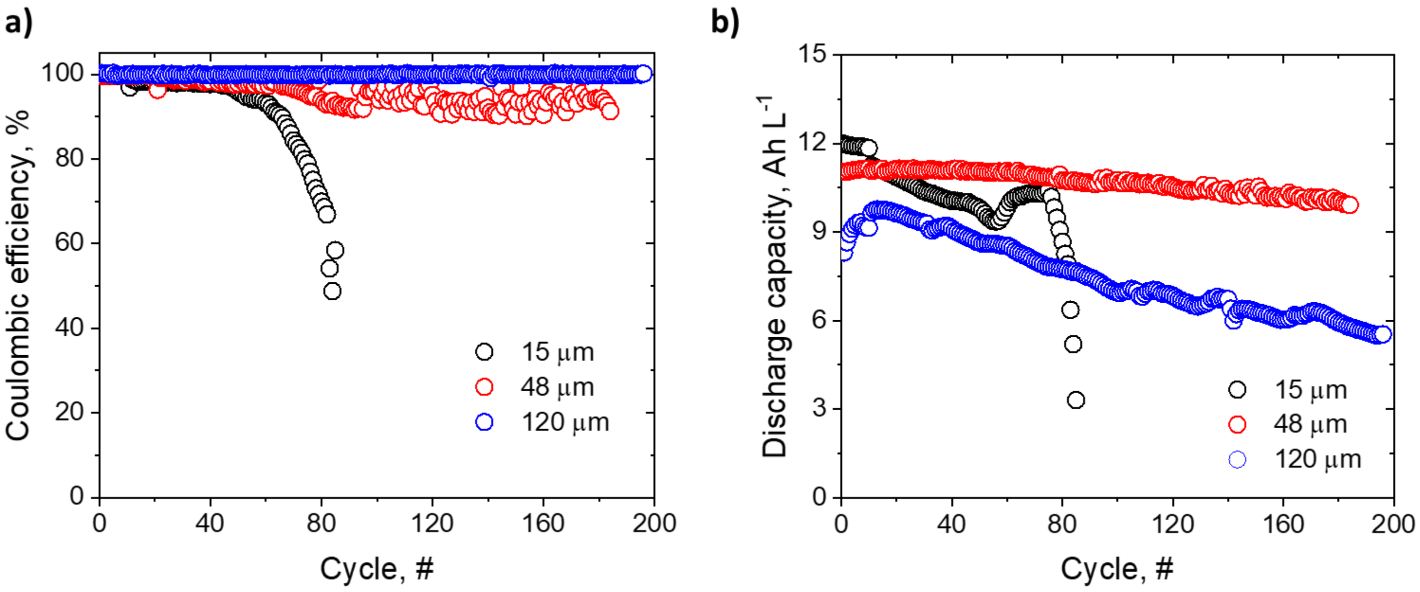


Fig. 3. Pressure and velocity distribution with serpentine flow field pattern a) pressure distribution in the channels and electrode b) velocity distribution in channels c) velocity distribution in the electrode.

Thank You

Polynitrile membrane



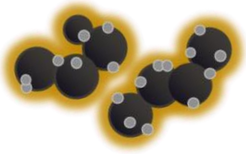
Alkaline and High Temperature Polymer Electrolyte Development

Sarah Eun Joo Park, MPA-11

Chemours company visit
5/24/2022

Development of polymer electrolytes

catalyst layer
ionomers



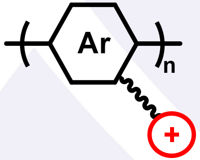
Hydrogen and fuel cell technologies

- Alkaline membrane fuel cells
- High temperature proton exchange membrane fuel cells
- Alkaline membrane water electrolyzers

Aqueous and non-aqueous redox flow batteries

Hydrocarbon polymers for electrolytes

- Design flexibility
- Versatile use in different pH/temperature environment
- High gas barrier properties

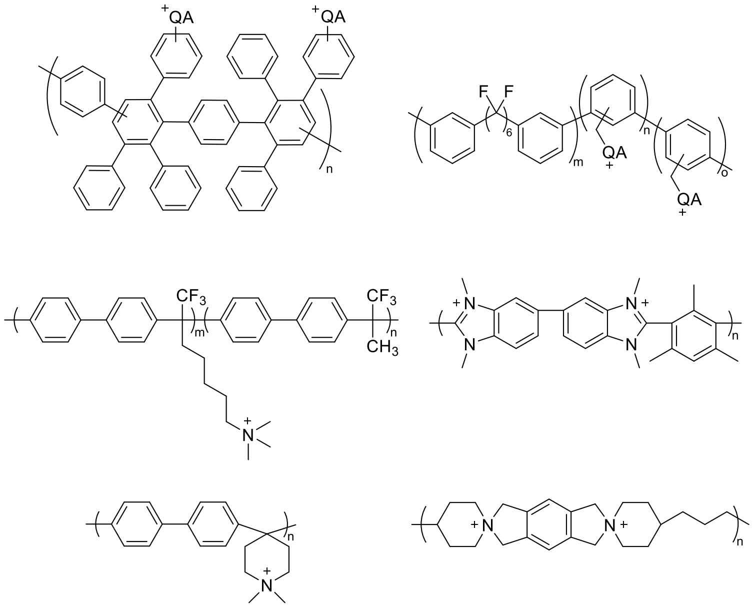


polymer backbone

cationic group

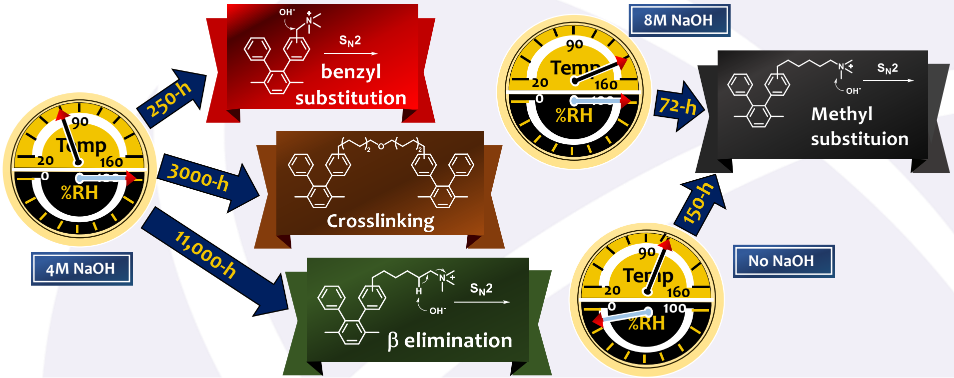
Alkaline stability of AEMs

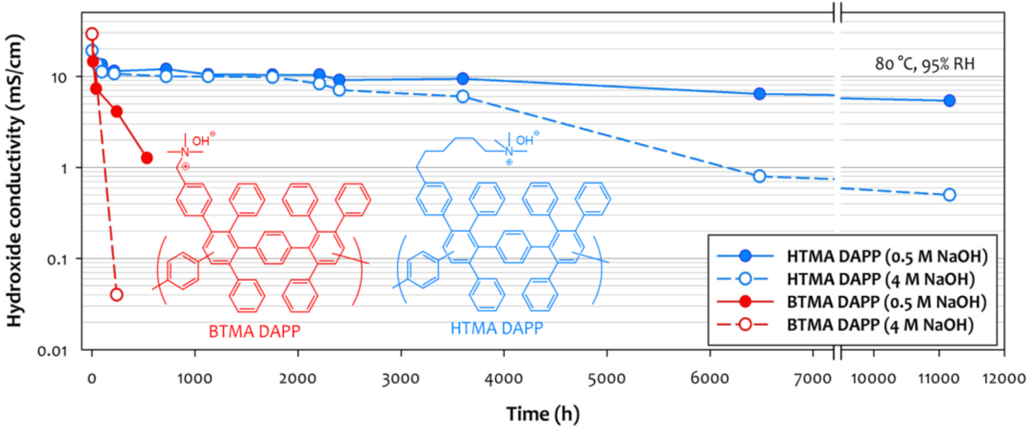
Aryl ether-free polyaromatics



Journal of Materials Chemistry A **2018**, *6* , 15456.

Degradation pathways of Diels-Alder Poly(phenylene)s under high pH



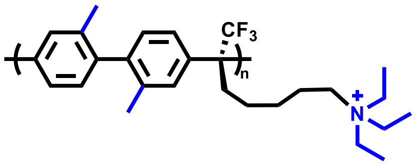


Macromolecules **2019**, *52*, 5419.

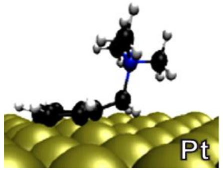
Los Alamos NATIONAL LABORATORY

Ionomers serving various functions

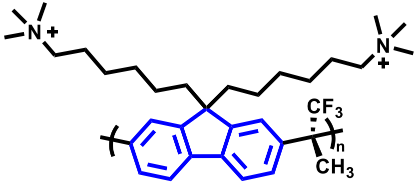
Increase H_2 permeability



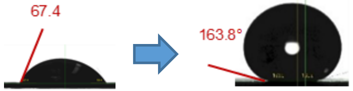
J. Mater. Chem. A **2019**, *7*, 25040
Patent pending 62/678832



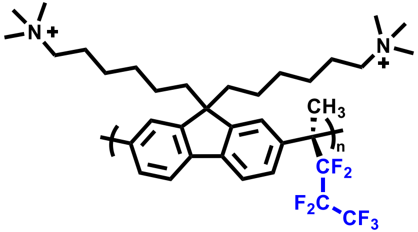
Minimize catalyst interaction



Energy Environ. Sci. **2018**, *11*, 3283
J. Mater. Chem. A **2020**, *8*, 14135

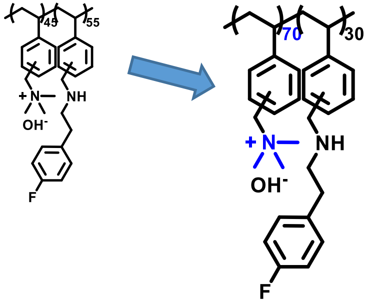


Increase hydrophobicity



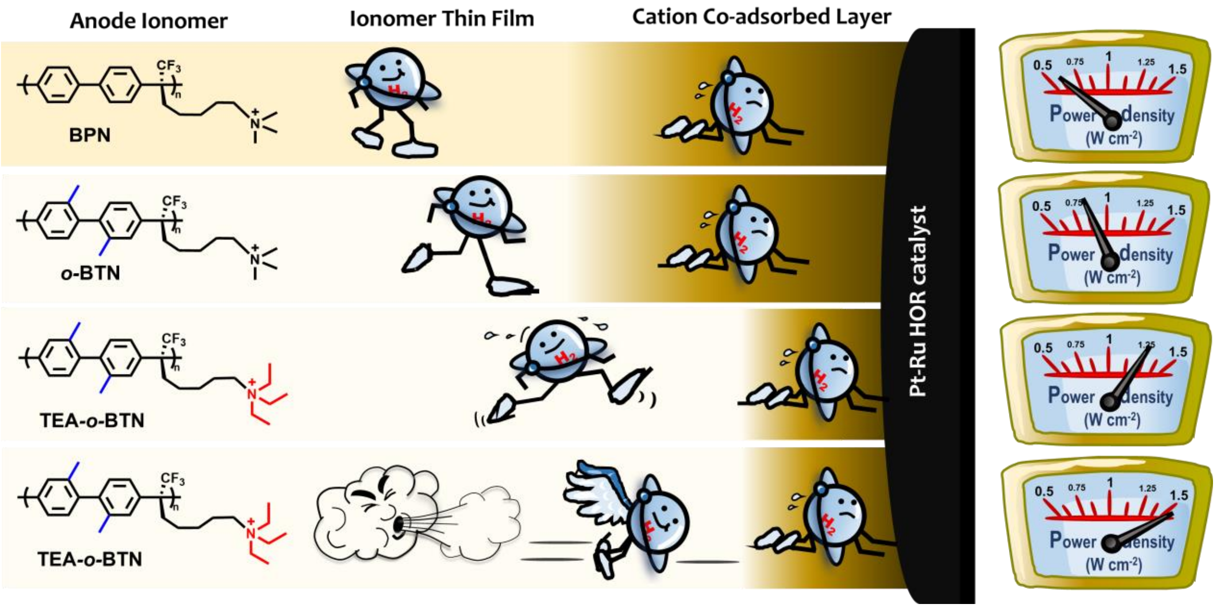
ACS Appl. Energy Mater. **2022**, *5*, 2663
Patent pending S167576

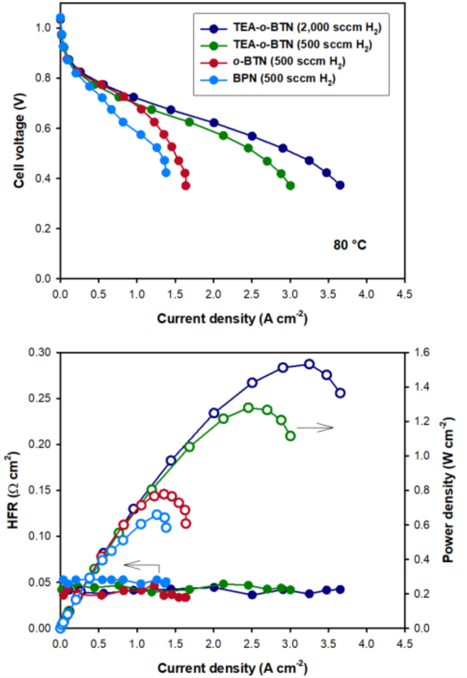
Control electrode pH



Nature Energy **2020**, *5*, 378

H_2 permeable alkaline ionomers



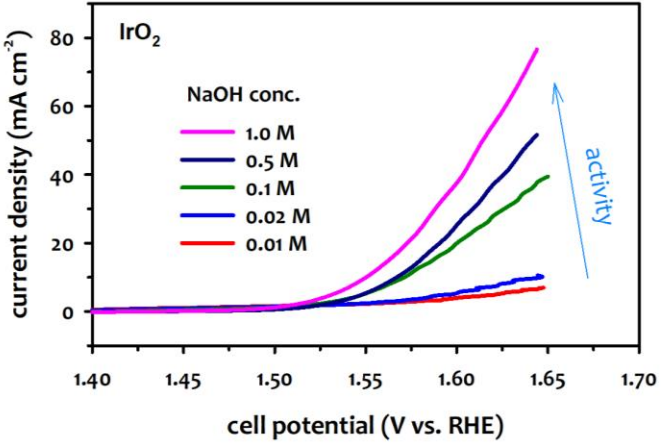


- Structural difference of backbone and cationic functional group for anode polymer electrolytes may improve hydrogen permeability and fuel cell performance.

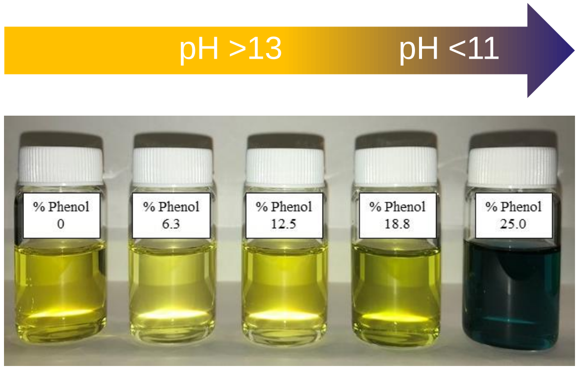
Journal of Material Chemistry A **2019**, *7*, 25040.

Ionomers for alkaline membrane water electrolyzers

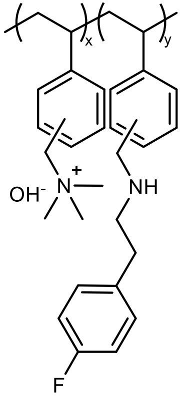
- Synthesis of quaternized ammonium functionalized ionomers having high IEC for anion exchange membrane water electrolysis



A high concentration of quaternary ammonium is required for the high activity of the hydrogen and oxygen evolution reactions.



Polyaromatic backbone have a detrimental impact by forming acidic phenols at high anode potentials.



TMA-45, IEC = 2.2 mequiv. g^{-1}
TMA-53, IEC = 2.6 mequiv. g^{-1}
TMA-62, IEC = 2.9 mequiv. g^{-1}
TMA-70, IEC = 3.3 mequiv. g^{-1}

Ionomers with high ammonium concentration was synthesized to demonstrate the record high H_2-generating current density of 2.7 A/cm^2 at 1.8 V.

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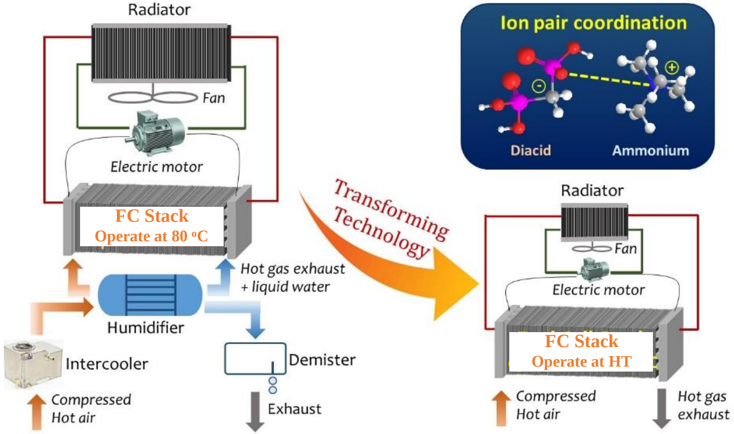
Nature Energy **2020**, *5*, 378-385.

HT-PEMFC (100-230 ºC) for Heavy-Duty Vehicles

- Easier thermal management
- Simplified water management
- Improved CO tolerance

▼ Simplified FC system with HT-PEMFC

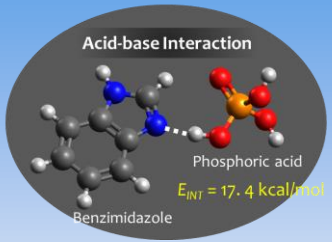


https://hydrogen-central.com/hydrogen-fuel-cell-truck-market-growth-information-trends/

- Need HT-PEM and ionomeric binder
- Adequate phosphoric acid management
  - retaining acid for proton conductivity
  - preventing acid flooding in electrodes

Progression of LANL's MEA development for HT-PEMFCs

Control
Phosphoric acid-PBI PEM
(1991 – present)

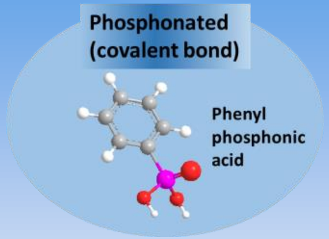


0.43 W cm^{-2} PPD

GEN 1
Ion-pair PEM
(2015-2016)

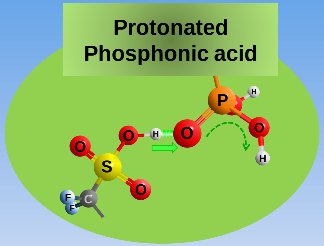
0.30 W cm^{-2} PPD

GEN 2
Phosphonated ionomer
(2017-2019)



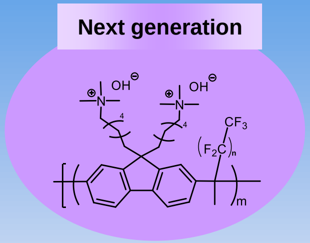
0.48 W cm^{-2} PPD

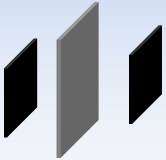
GEN 3
Protonated ionomer
(2020-2021)



0.80 W cm^{-2} PPD

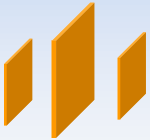
GEN 4
Fluorinated ion-pair
ionomer (2022-)





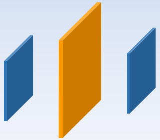
PA-PBI PEM
PTFE binder

Improved
water tolerance



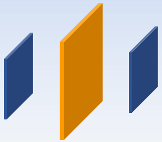
Ion-pair PEM
Ion-pair
ionomer

Improved
water tolerance
& performance



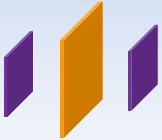
Ion-pair PEM
Phosphonated
ionomer

Improved
conductivity



Ion-pair PEM
Protonated
ionomer

Increased
hydrophobicity



Ion-pair PEM
F-ion-pair
ionomer

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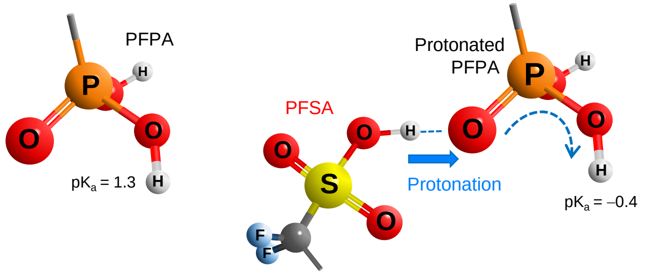
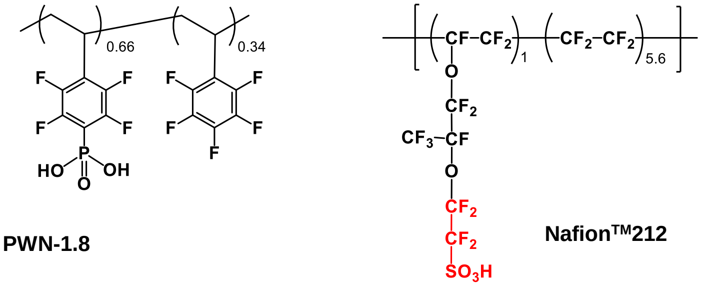
Protonation of phosphonic acids

Protonation of phosphonic acids



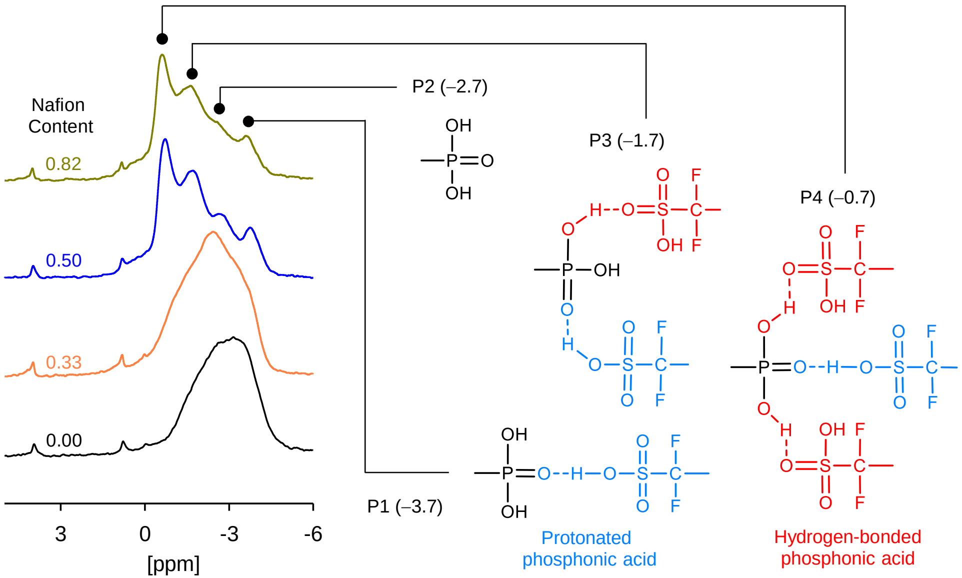
Ionomer system



PWN-1.8

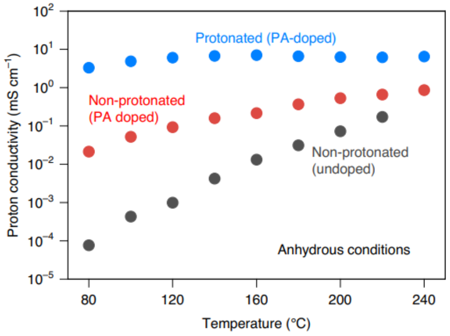
Nafion^{TM}212

^{31}P NMR spectra of hydrogen-bonded and protonated phosphonic acids



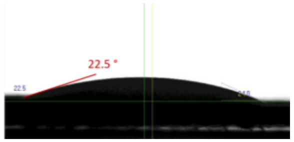
Impact of protonation on the performance of HT-PEMFCs

Proton Conductivity ↑

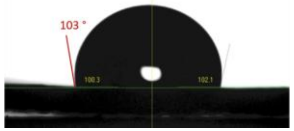


Hydrophobicity ↑

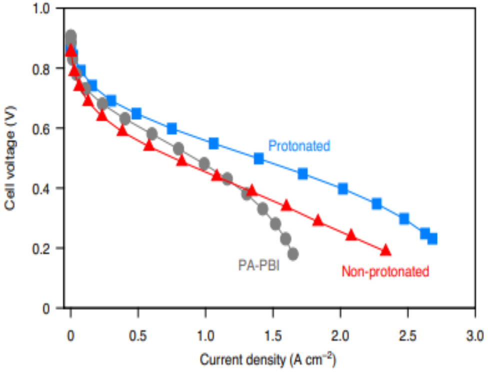
Non-protonated

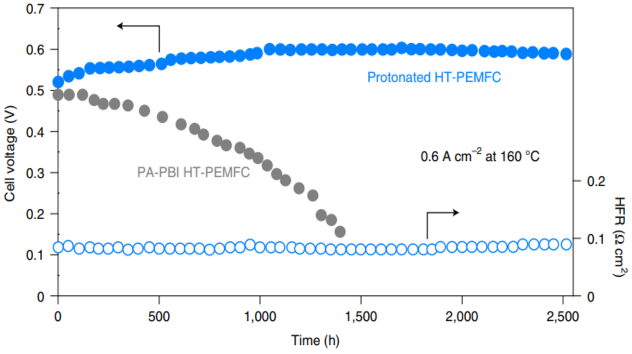


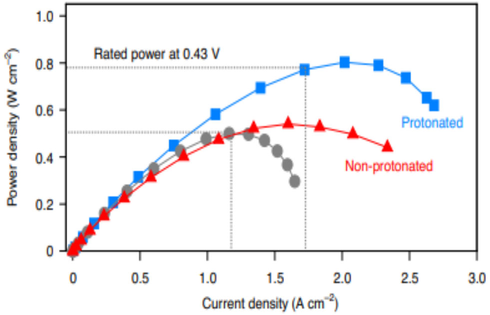
Protonated



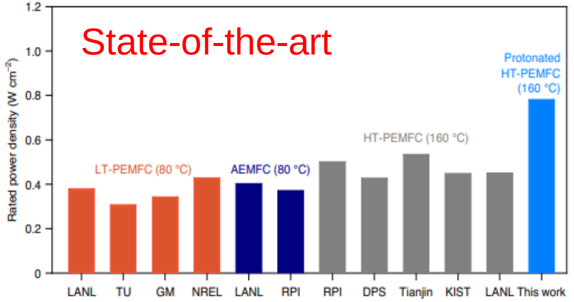
Performance and Durability ↑







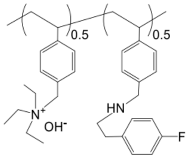
State-of-the-art

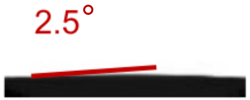


Nature Energy **2022**, *7*, 248.

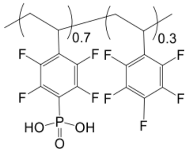
Hydrophobic Ionomer Development

Control hydrophobicity of electrode with poly(fluorene) ionomers

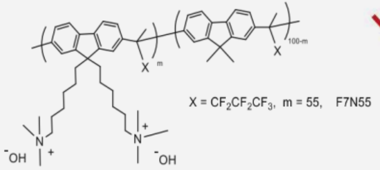


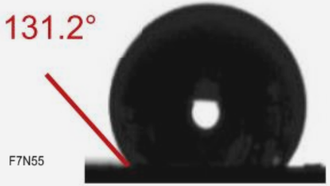


QASOH (2016)

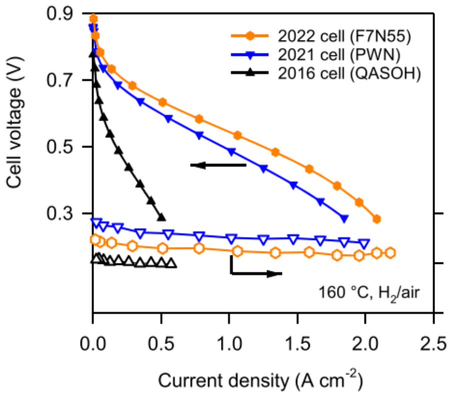


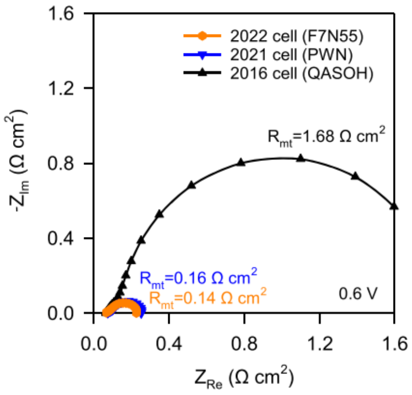
PWN (2021)





F7N55 (2022)





- ✓ Hydrophobicity of electrode was controlled with different ionomers.
- ✓ F7N55 can hold more PA with ion-pair interaction but also prevent an electrode flooding effect with its hydrophobicity.
  → Higher performance

ACS Applied Energy Materials **2022**, *5*, 2663.

Performance and Durability Investigation of Thin, Low Crossover Proton Exchange Membranes for Water Electrolyzers

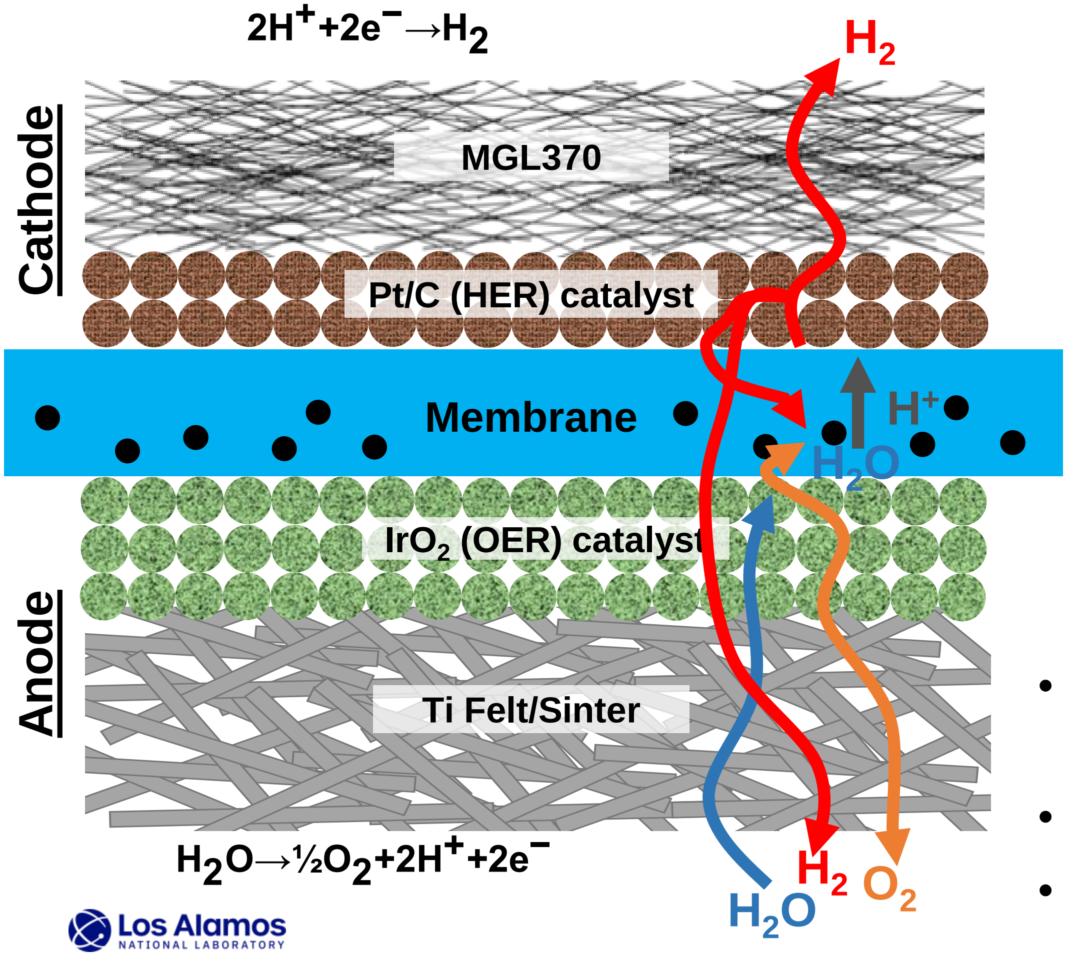
LANL: Kaustubh Khedekar [a], Christopher Evan Van Pelt [a], Rangachary Mukundan [a], Rod Borup [a], Siddharth Komini Babu [a]

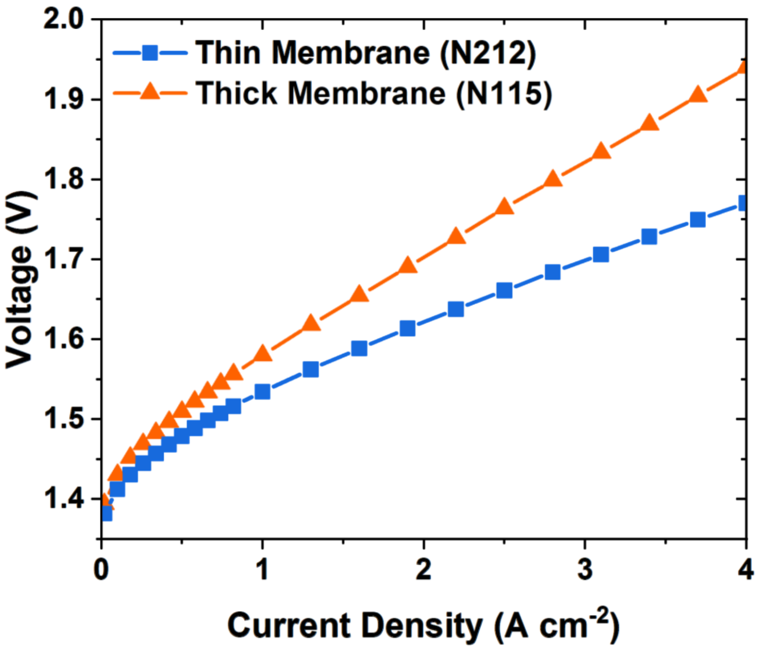
Chemours: Andrew M. Park [b], Ryan Gebhardt [b]

DOE Project Award #DE-EE0008836

05/24/2022

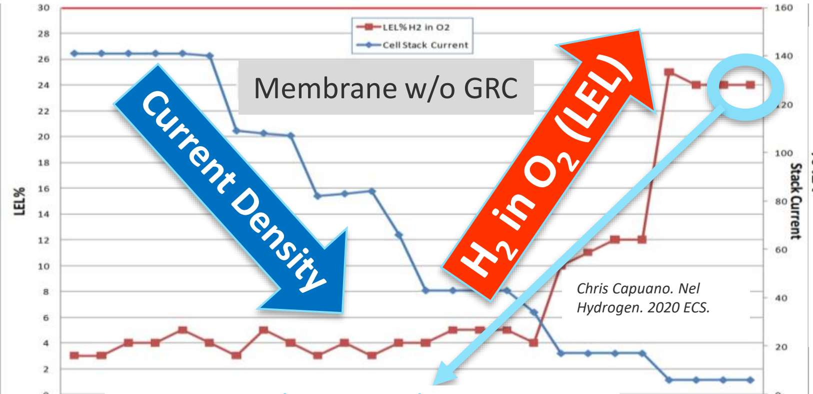
Hydrogen Crossover



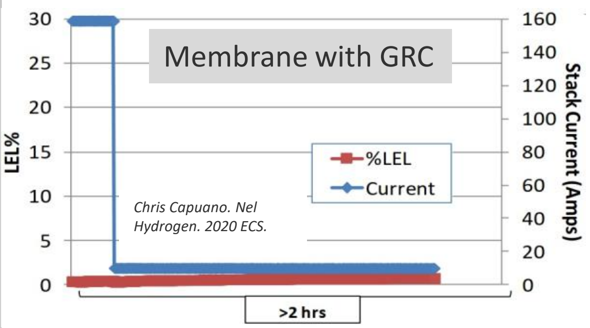


- Thin membranes are required to meet DOE 111 target.
- Thin membranes have high crossover
- Thick membranes reduces efficiency

Approach – Innovation: Combination of Several Benefits Into One Membrane

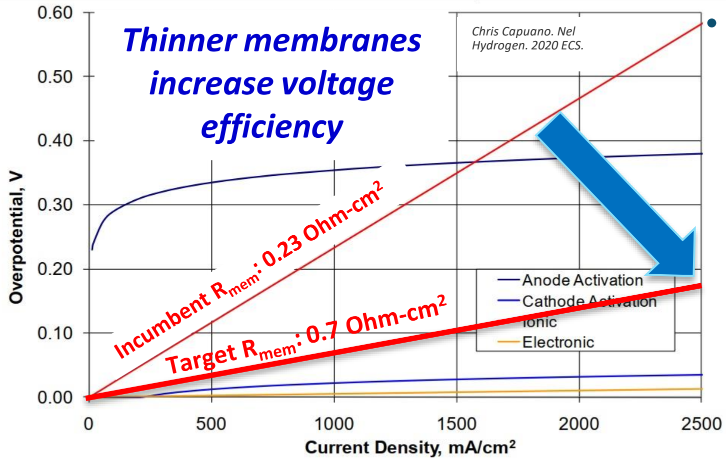


~1% H_2 in O_2 (25% of LEL) without GRC

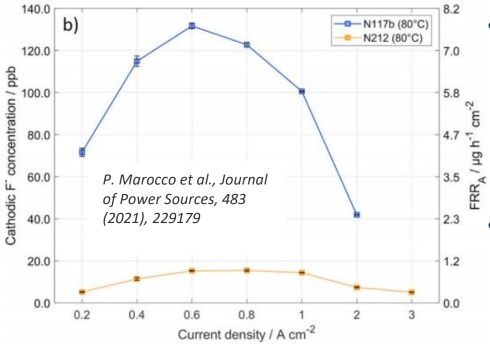


- **Pursuit of cheap electricity (feedstock) will require usage of intermittent energy**
- **Current density will follow varying electrical load**
- **Low current density results in high H_2 in O_2 content (safety concern – LEL = 4%)**

GRCs enable safe stack operation for load-following applications, especially at high ΔP with a thin membrane



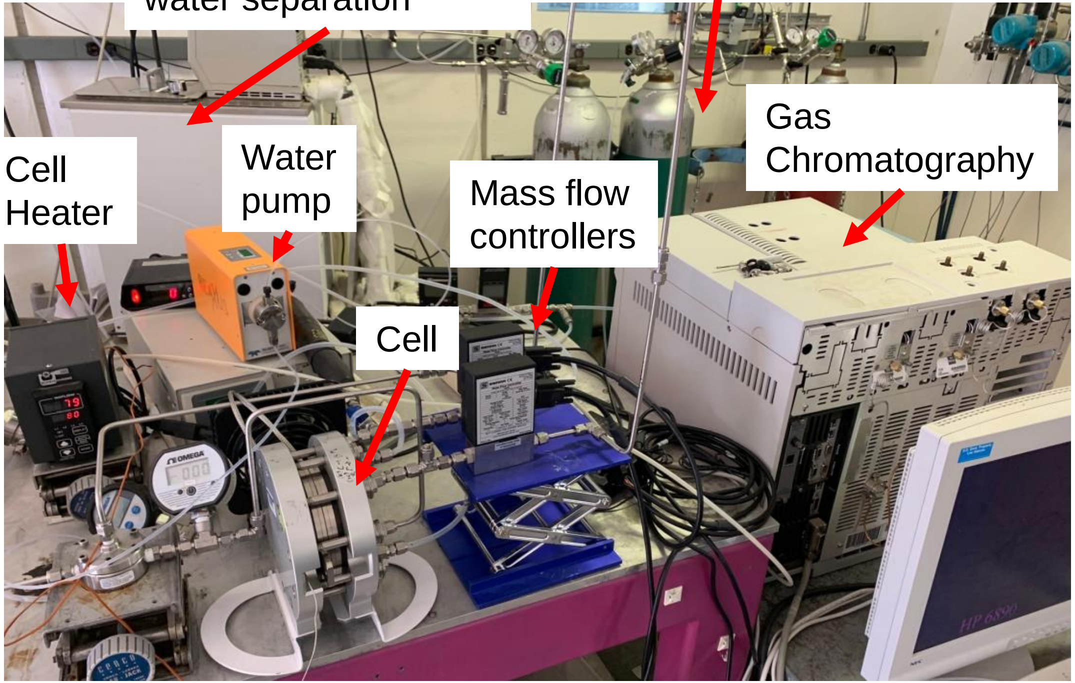
- **Reinforcing thin membranes is preferred for several benefits:**
  1. **Handleability (especially at scale)**
  2. **Mechanical Properties**
  3. **Low x-y expansion**
  4. **Enables low EW ionomers**

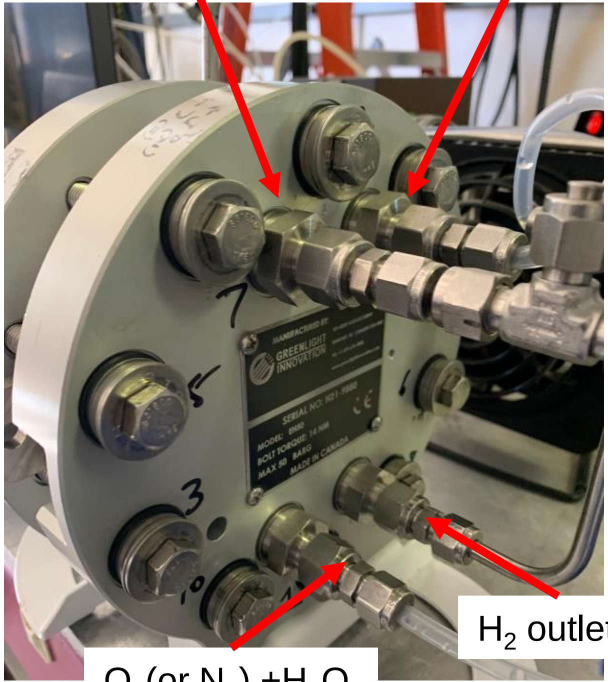


- **Fluoride ions have been quantified in PEMWE cell effluent**
- **Fluoride loss exacerbated at high temps**

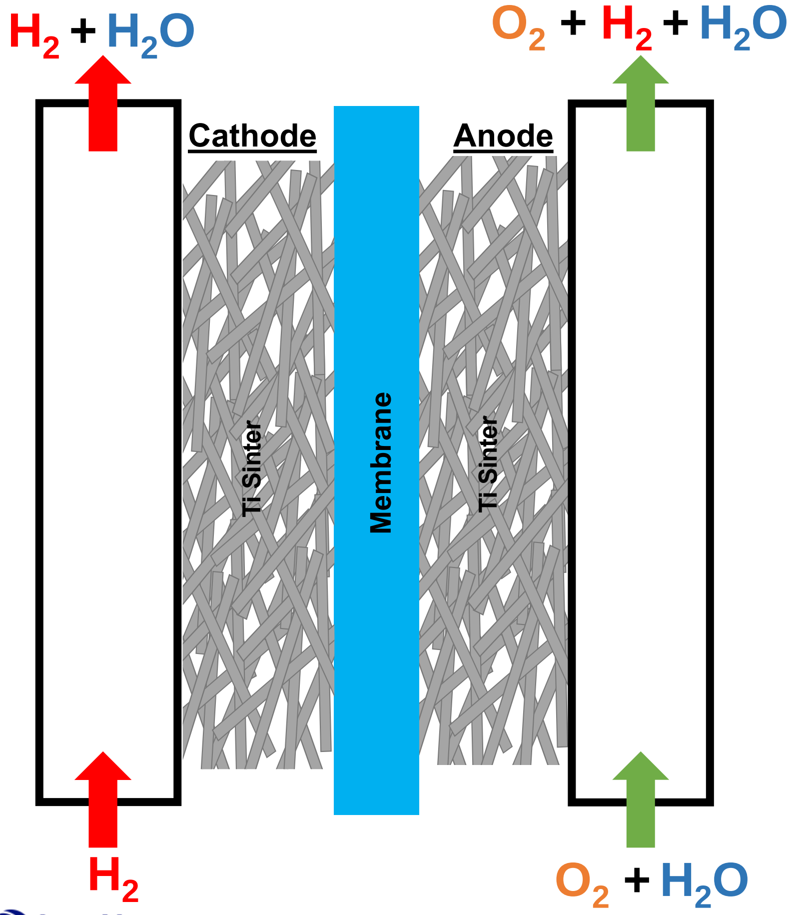
Radical scavengers will be investigated to understand impact on PEMWE degradation

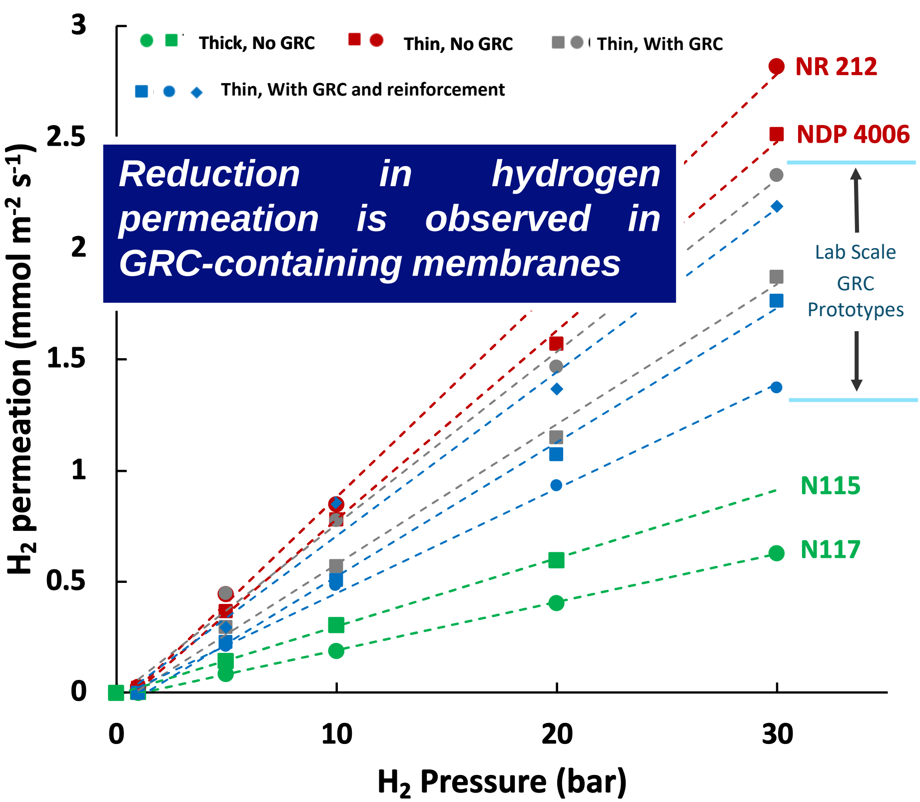
Experimental Setup





Ex-situ H_2 Permeation Measurement



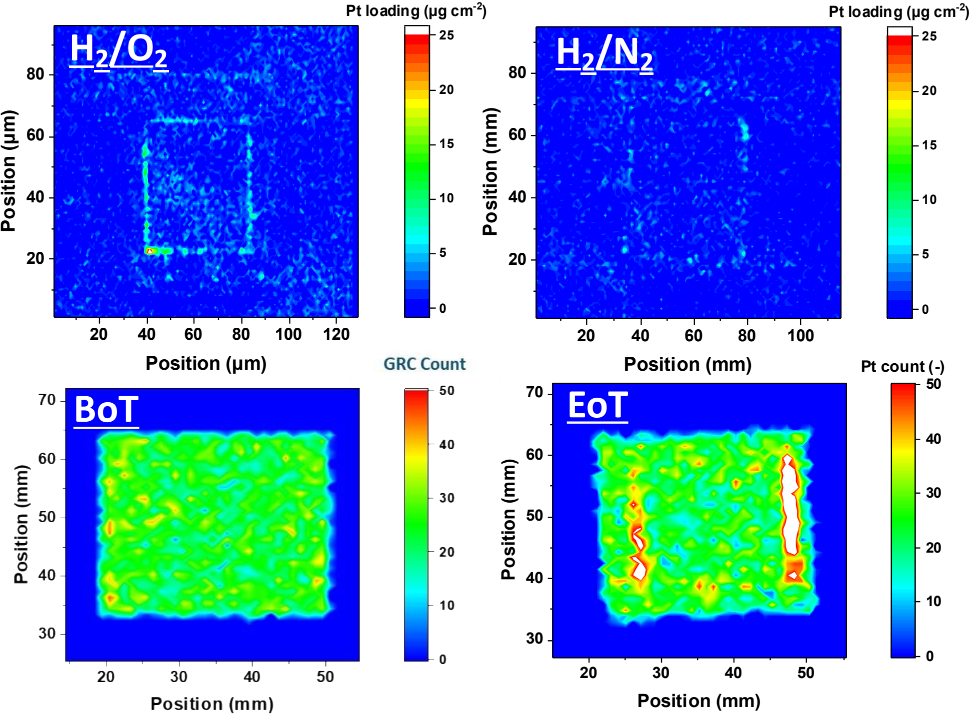


Reduction in hydrogen permeation is observed in GRC-containing membranes

Active area: 45 cm^2, Cell temperature: 80 °C,
O_2 partial pressure: 1 atm, flow rate 300 sccm

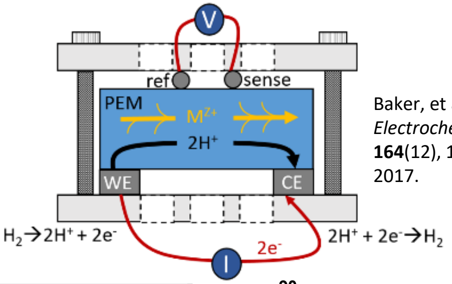
GRC and Radical Scavenger Migration

GRC Migration

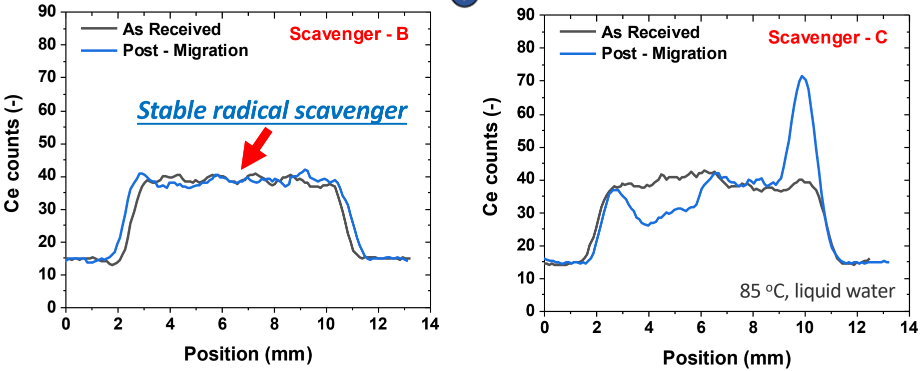


Cell temp: 65 ˚C, Cathode: Dry H_2 at 2.75 kPa, Anode: N_2/O_2 at 300 % RH and 0.75 kPa + 3 ml/min H_2O

Radical Scavenger Migration

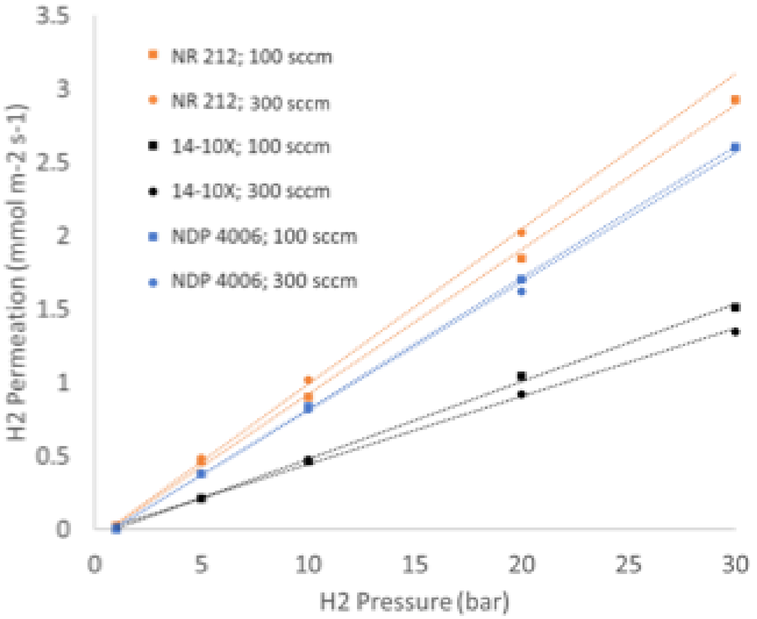


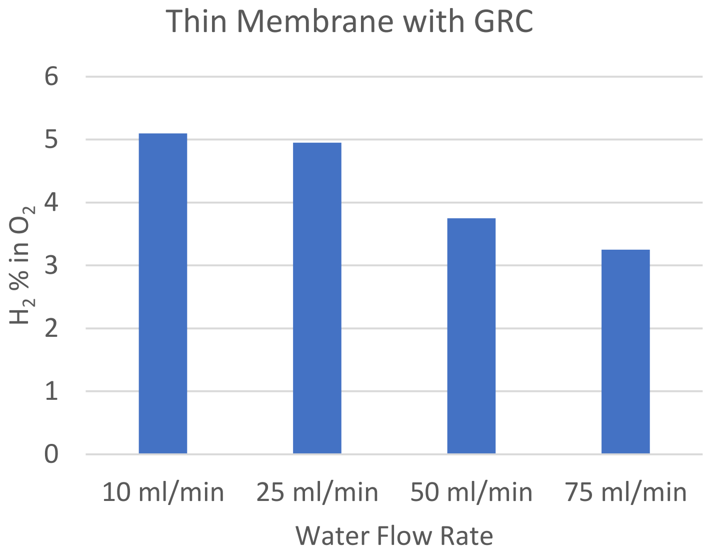
Baker, et al., *J. Electrochem. Soc.*, **164**(12), 1272-1278, 2017.



XRF capability to map in-situ movement of GRC and scavengers will be critical to ensure durability of membrane

Ex-situ H_2 Permeation Measurement





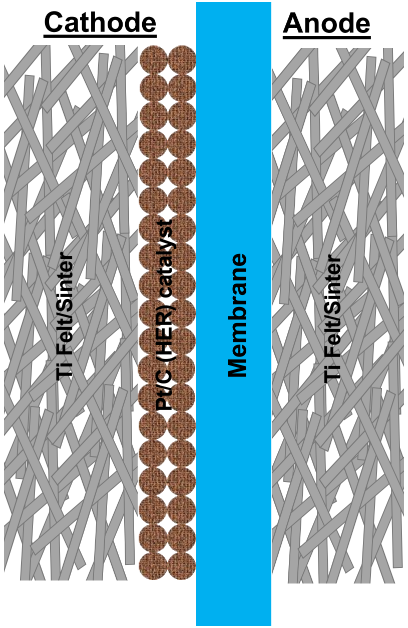
- Effect of current density is simulated by varying flow rate, where flow rate corresponds to gas produced in-operando
  - 100 sccm – 0.32 A cm^{-2} and 300 sccm – 0.96 A cm^{-2}
- At higher flow rates, H_2 in O_2 content is significantly lower due to dilution of crossover H_2 by higher O_2 flow rate.

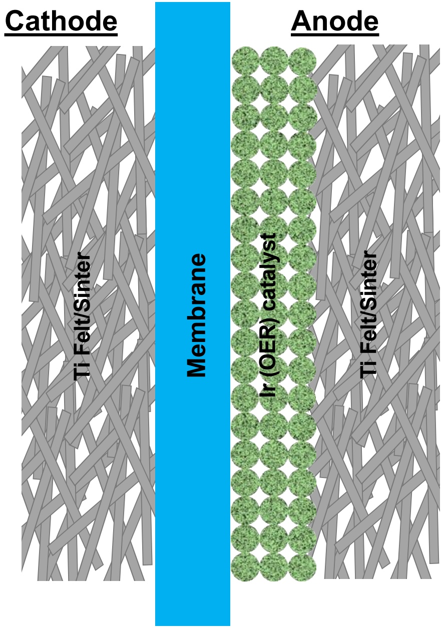
- Effect of flow rate on crossover observed
- Ongoing study to deconvolute the effect of GRC activation vs. thickness increase due to swelling

Ex-situ setup enables study of operating condition effect on H_2 crossover

On-Going Work

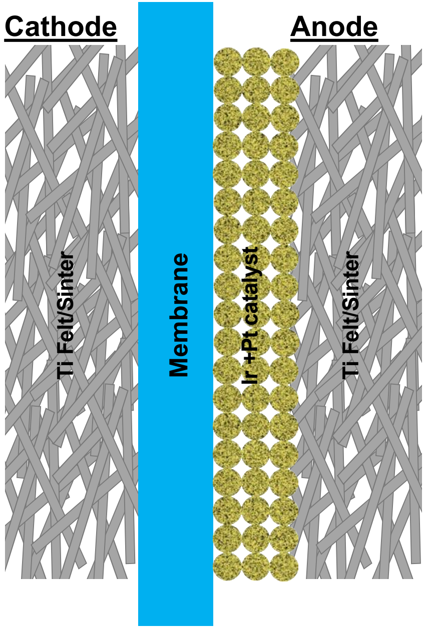
Effect of Catalyst Layer



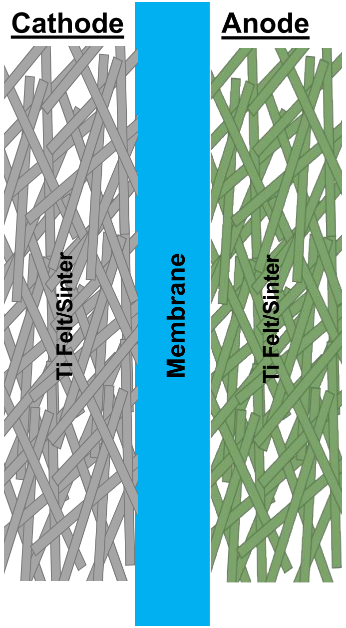


Placement of GRC

GRC in anode CL



GRC in anode PTL



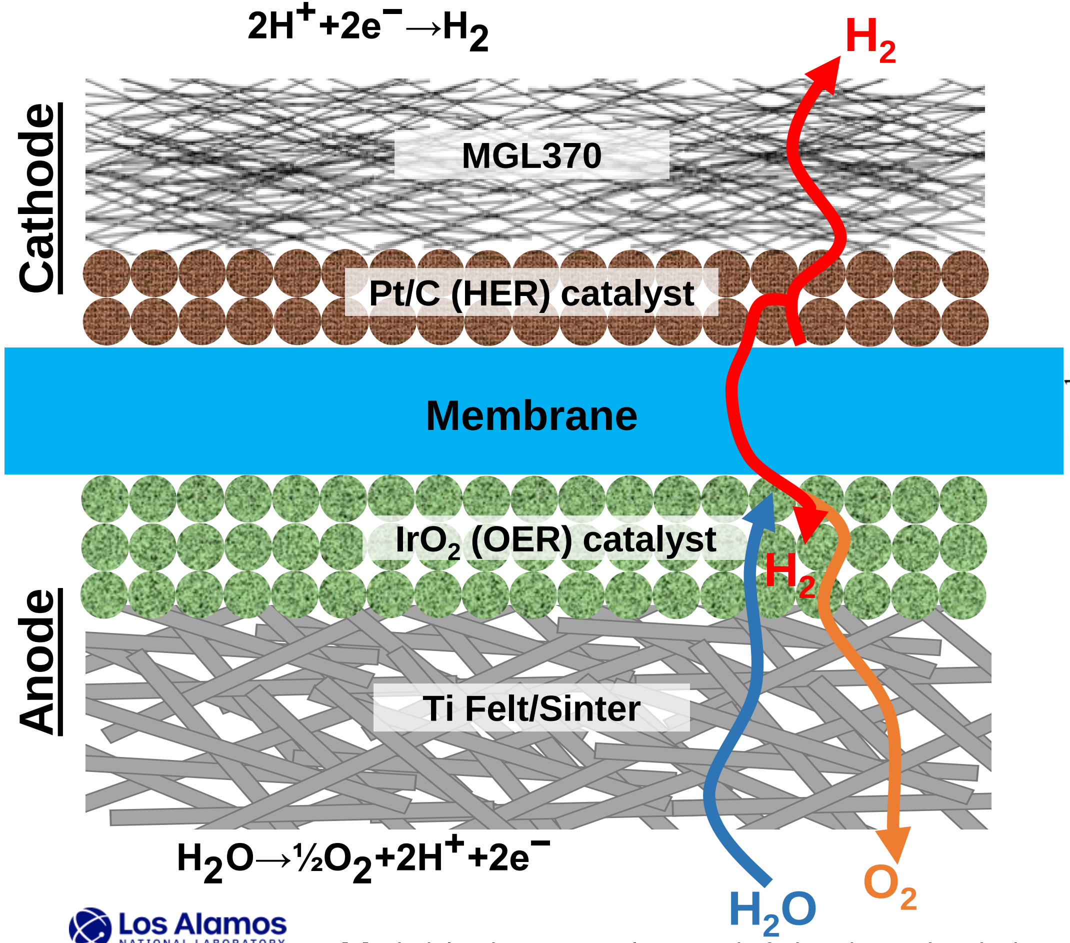
- *Utilizing ex-situ setup to study changes to H_2 permeation due to anode and cathode catalyst layer separately*
- *H2 crossover change due to placement of GRC and Pt in components*

H2NEW Consortium: Durability and AST of PEM Water Electrolyzers

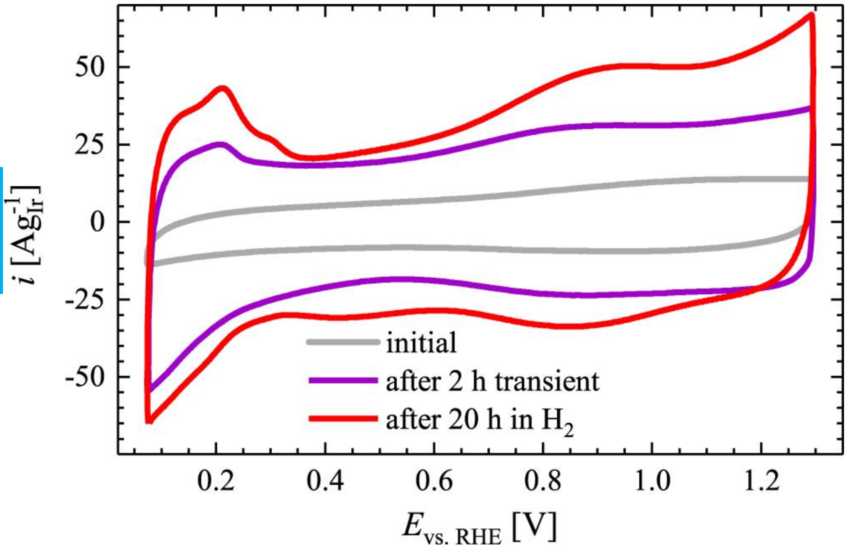
Abdurrahman Yilmaz, Xiaoxiao Qiao, Kui Li, Siddharth Komini Babu, Jacob S. Spendelow, Rangachary Mukundan

Los Alamos National Laboratory

Degradation due to Hydrogen Crossover

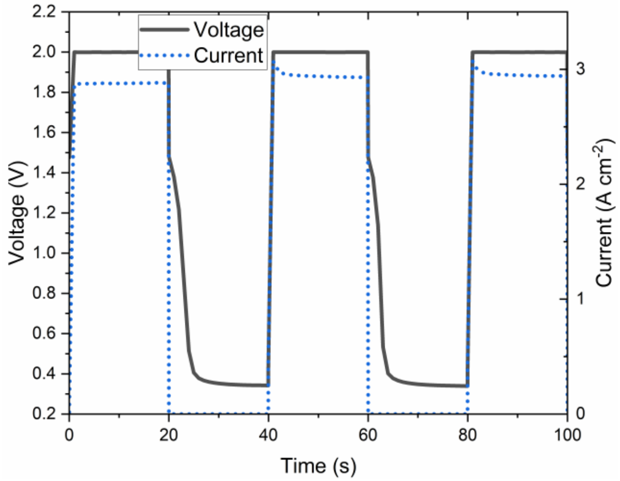


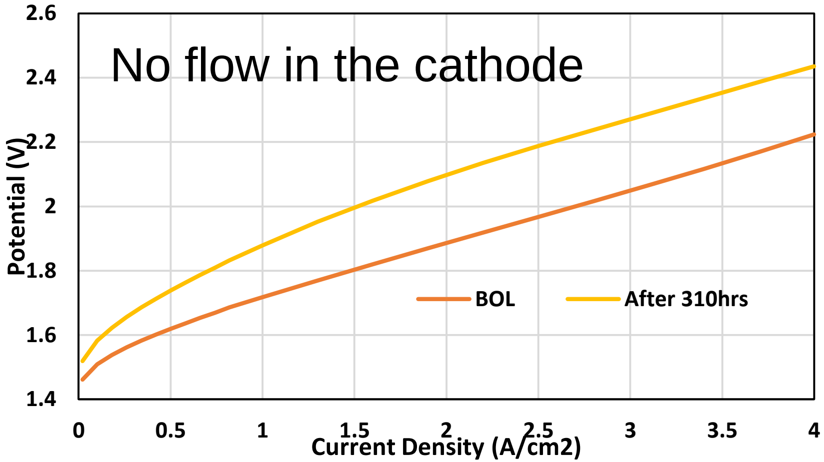
H_2 in Anode reduces IrO_2 [1]

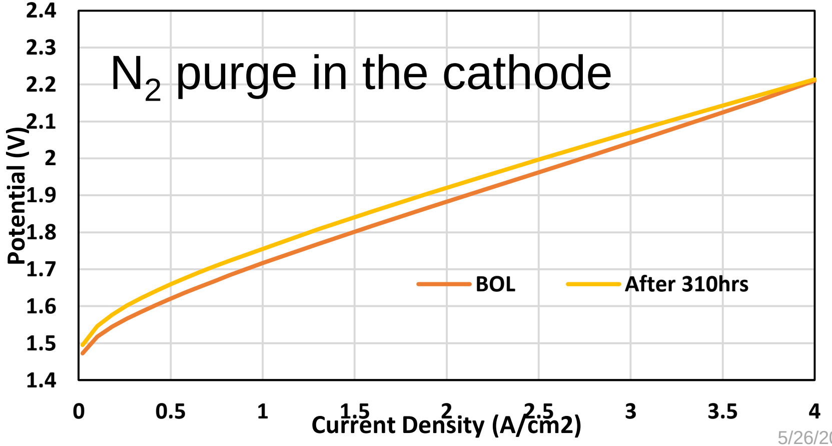


[1] Rheinländer, P.J. et al. *Journal of The Electrochemical Society*, *168*(2), p.024511, 2021.

Anode Catalyst AST



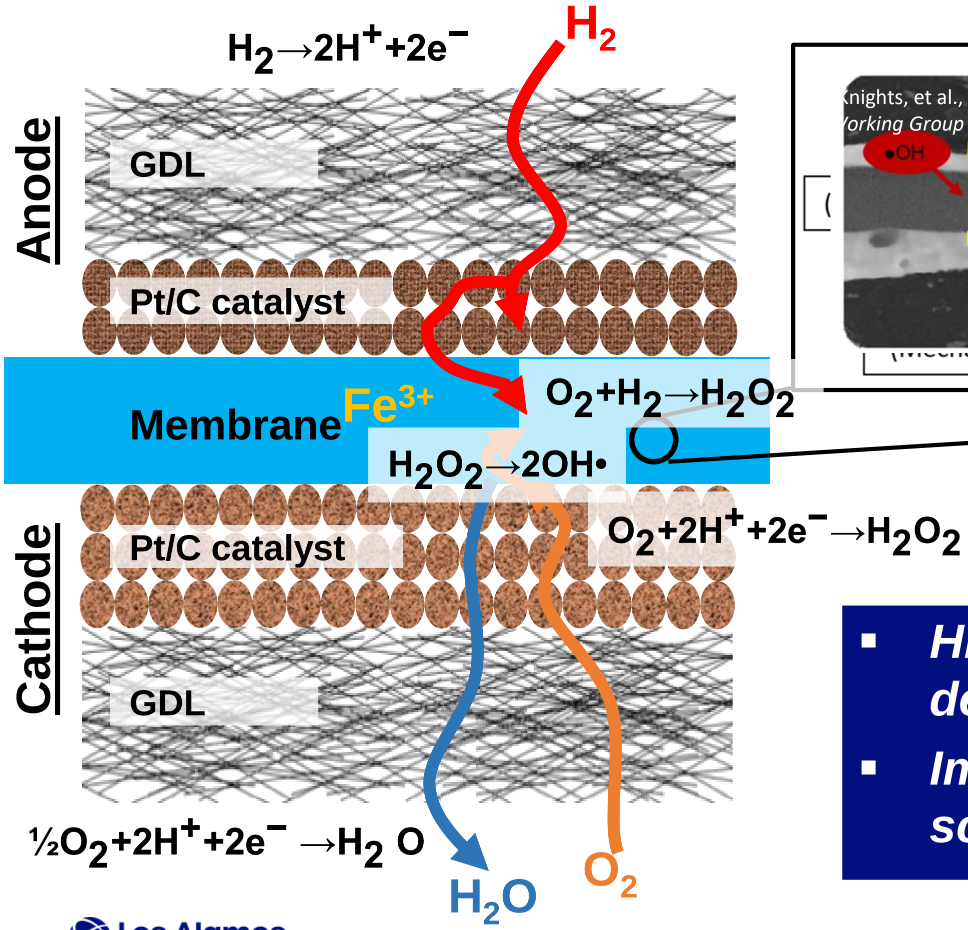


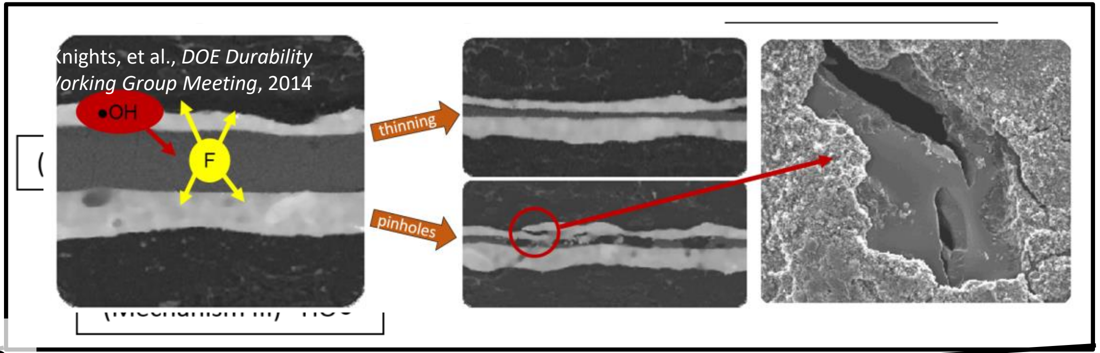


- ***Reducing the H_2 crossover by depolarizing the electrode through N_2 purge improves durability***
- ***Use of GRC in the membranes could enable improvement in catalyst durability***

Los Alamos NATIONAL LABORATORY

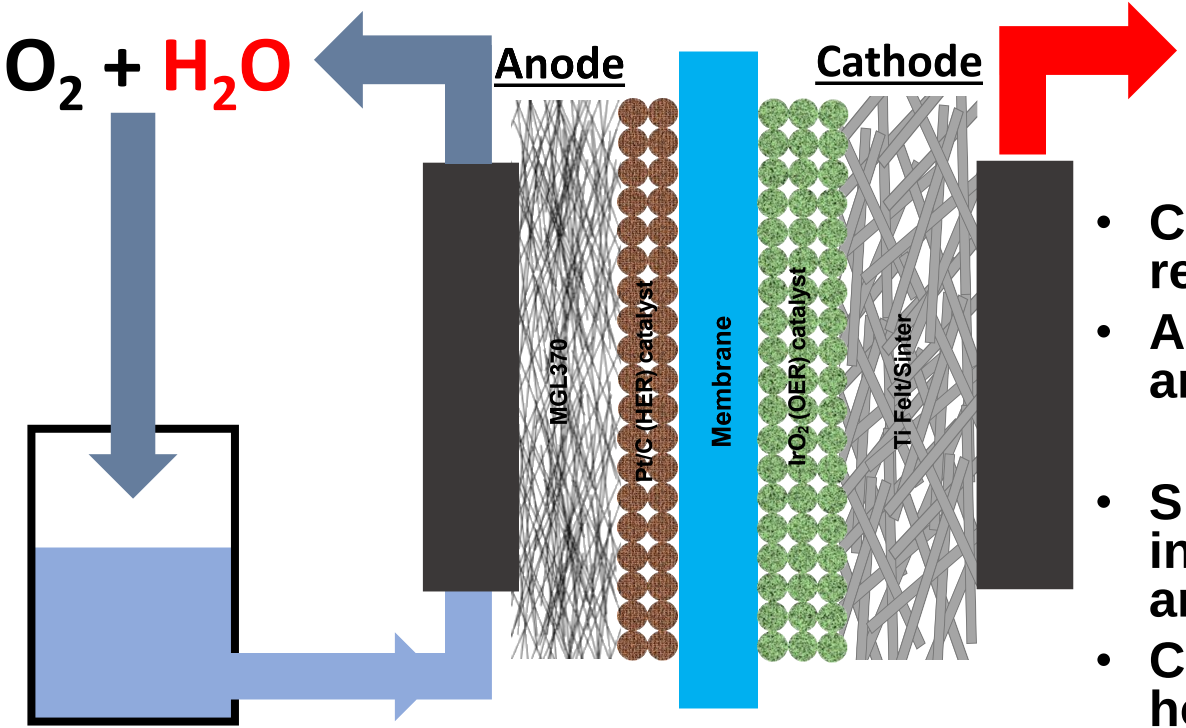
Chemical Degradation of PEM in Fuel Cells





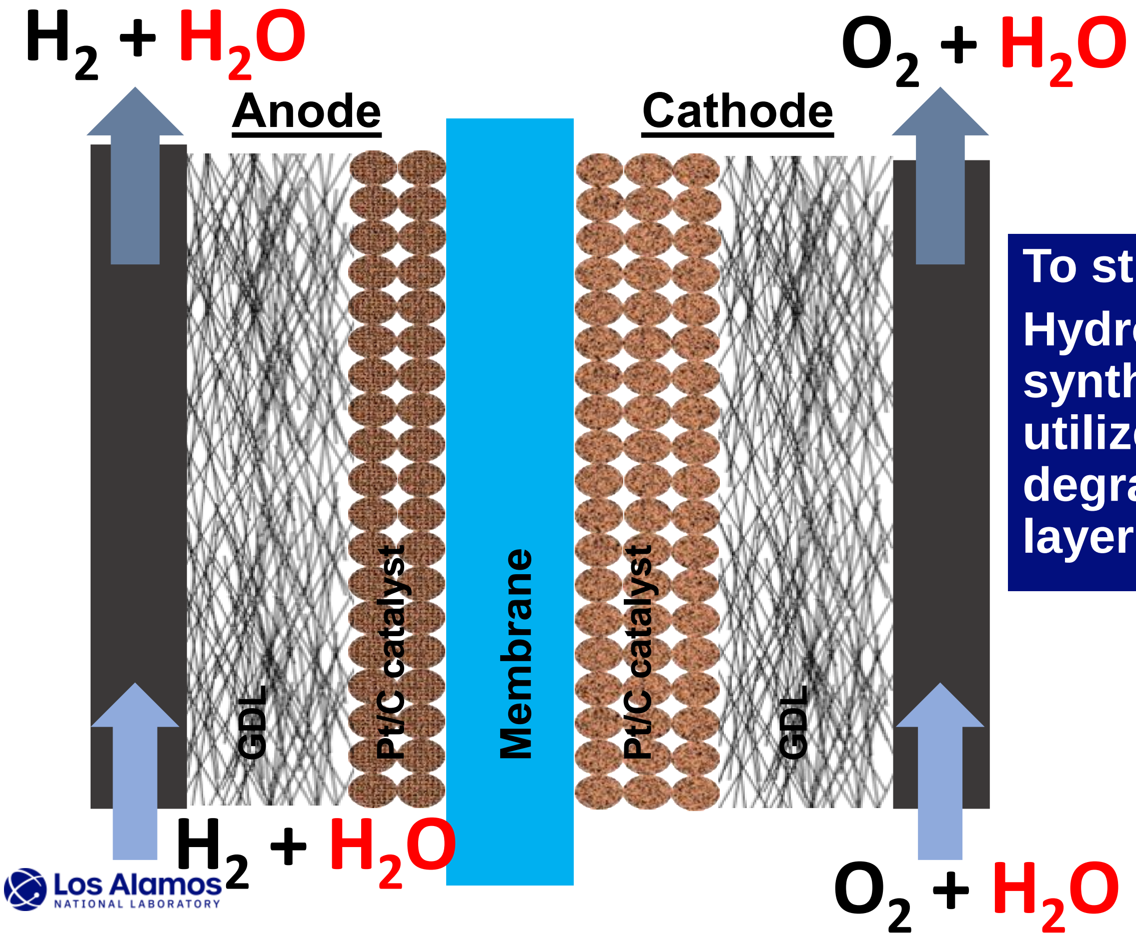
- *High temperature and low RH increased degradation of PEM in fuel cells*
- *Improve durability through radical scavengers in MEA*

Experimental Setup



- Cathode water collected at regular intervals
- Anode water recirculated and analyzed at the end of test
- Simulated OCV: 200 sccm H_2 in cathode and O_2 +H_2O in anode
- Constant 0.6 A cm^{-2} current hold

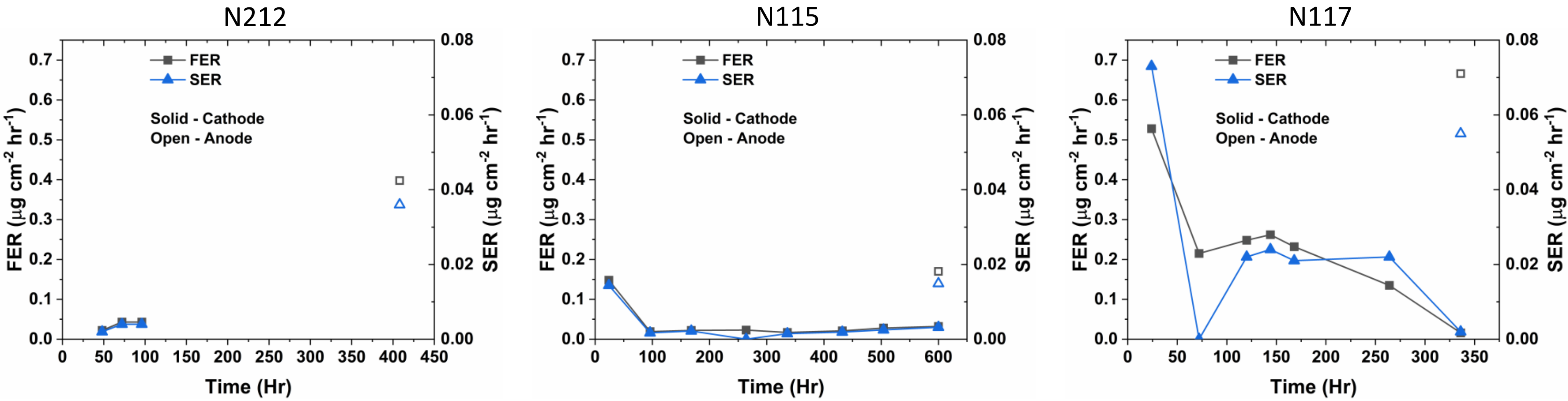
Ionomer Degradation



To study effect of HOPI in cathode:

Hydrocarbon membranes synthesized at LANL will be utilized to separate the degradation of ionomer in catalyst layer vs. membrane

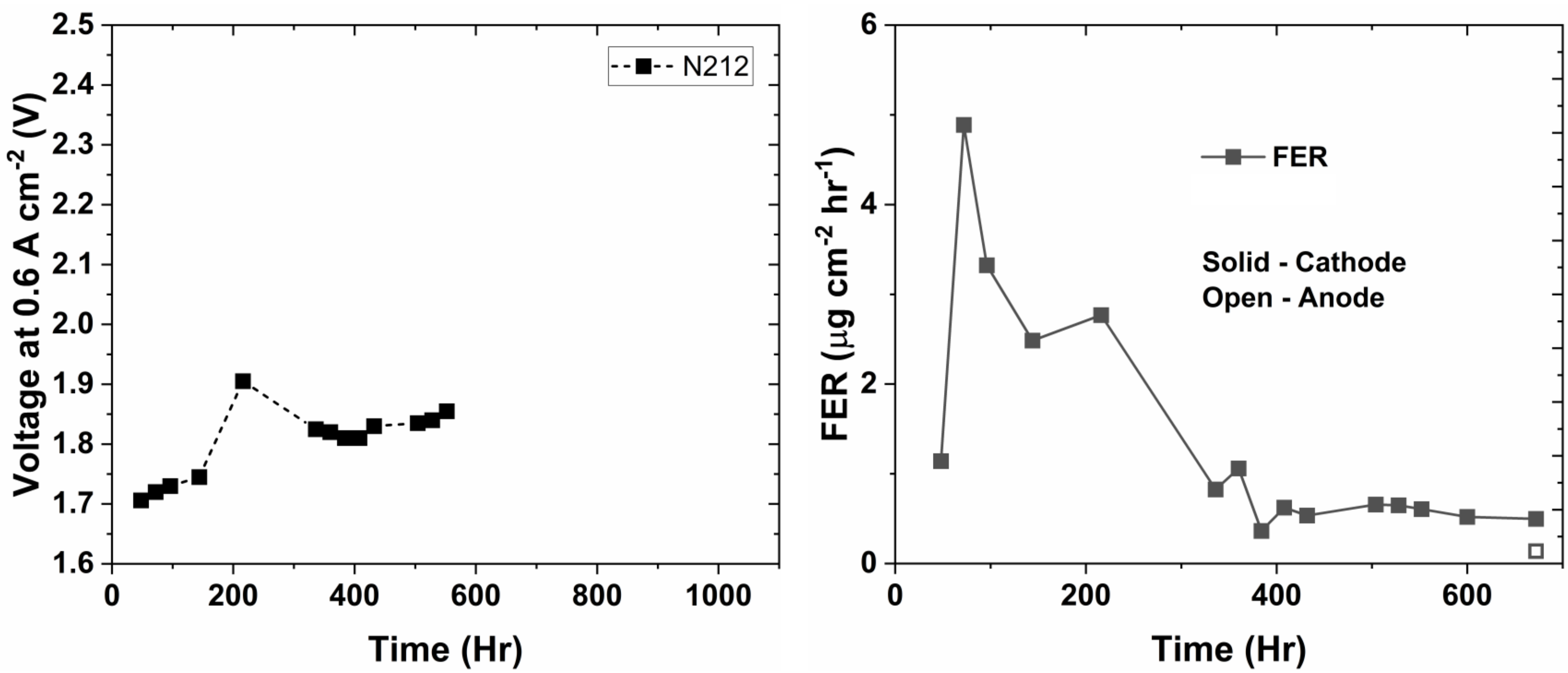
Membrane AST at Simulated OCV



- **Low FER in both anode and cathode**
  - **Anode FER higher than cathode FER**
- **FER**
  - **increases with initial fluoride inventory**
  - **decreases with decreasing crossover**

Cathode: 0.4 mg cm^{-2} IrO_2 (Alfa Aesar)
Anode: 0.1 mg cm^{-2} Pt/C (TEC10V20E)
Cell Temperature: 80 °C
Active area: 50 cm^2

Constant Current Density Hold – N212



- *At constant current density hold cathode FER is greater than anode FER*
- *FER is initially high but stable after 300 hours of testing*

Summary

- FER a balance between the crossover and material inventory

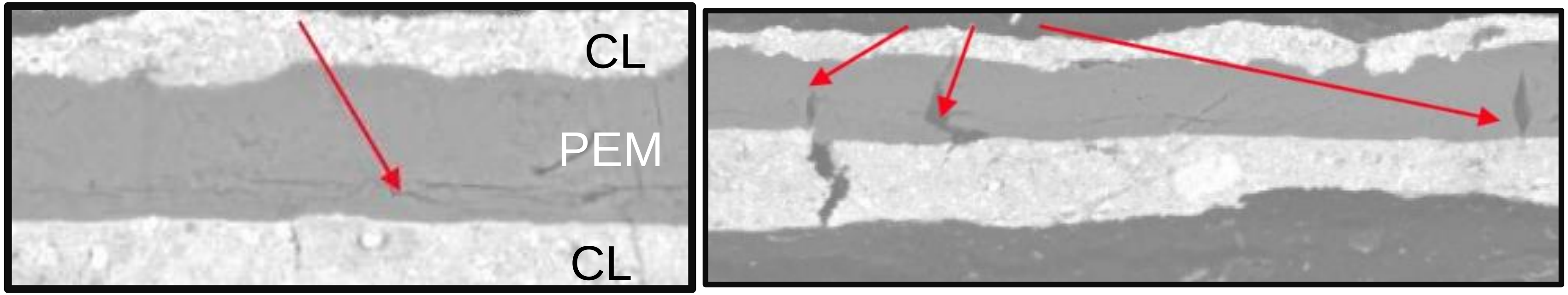
- FER in cathode higher than anode

- On going work to understand effect of crossover
  - H_2 crossover vs. O_2 crossover
  - Cross-over at low current density and high pressure

- Both catalyst and membrane degradation could be mitigated by utilizing membranes with GRC

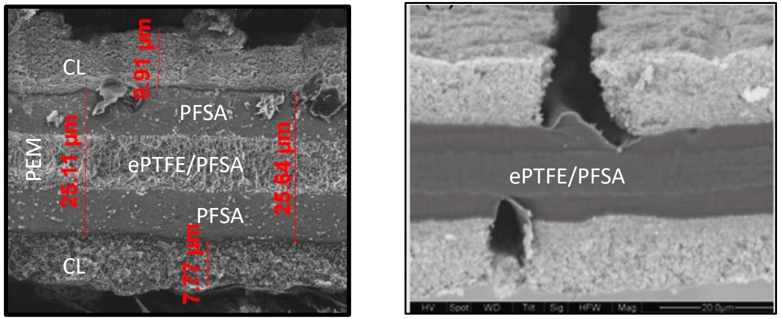
Membrane Mechanical Stability

Mechanical Failure in PFSA

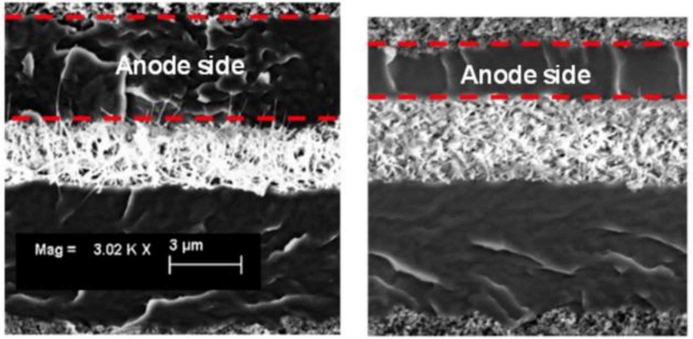


R. Mukundan, *U.S. DOE FCT Program Annual Merit Review*. 2014.

Mechanical PEM reinforcement improves strength and fracture toughness



C. S. Gittleman, et al., in *Polymer Electrolyte Fuel Cell Degradation*, 2011.



Zhang, J.,. *Journal of The Electrochemical Society*, *168*(2), p.024520.

- **Study effect of pressure change and membrane swelling on mechanical degradation**

Electrolyzer AST Working Group

- Led by Rangachary Mukundan
- Experts from National Labs, Industry, DOE, and Academia

National Labs:
NREL: Bryan Pivovar, Shaun Alia, Guido Bender, Mike Ulsh
LANL: Rangachary Mukundan, Siddharth Komini Babu
LBNL: Ahmet Kusoglu
ANL: Debbie Myers, Rajesh Ahluwalia
ORNL: Haoran Yu

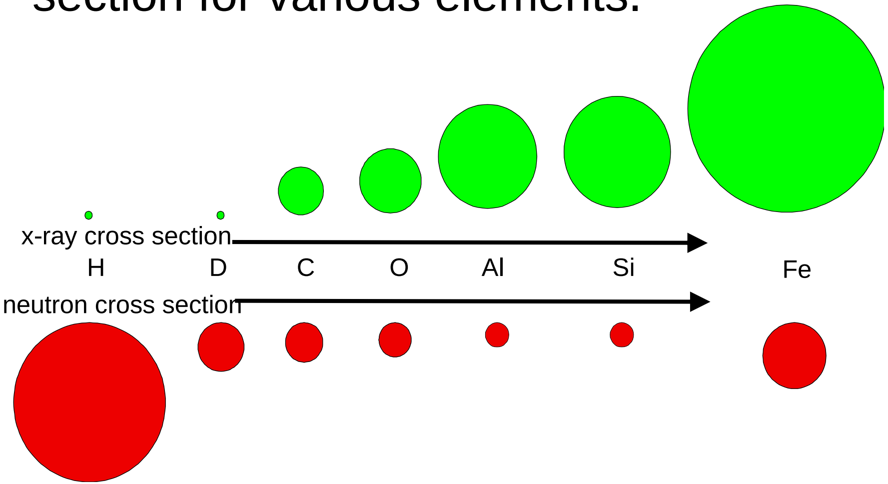
DOE:
Dave Peterson
Will Gibbons

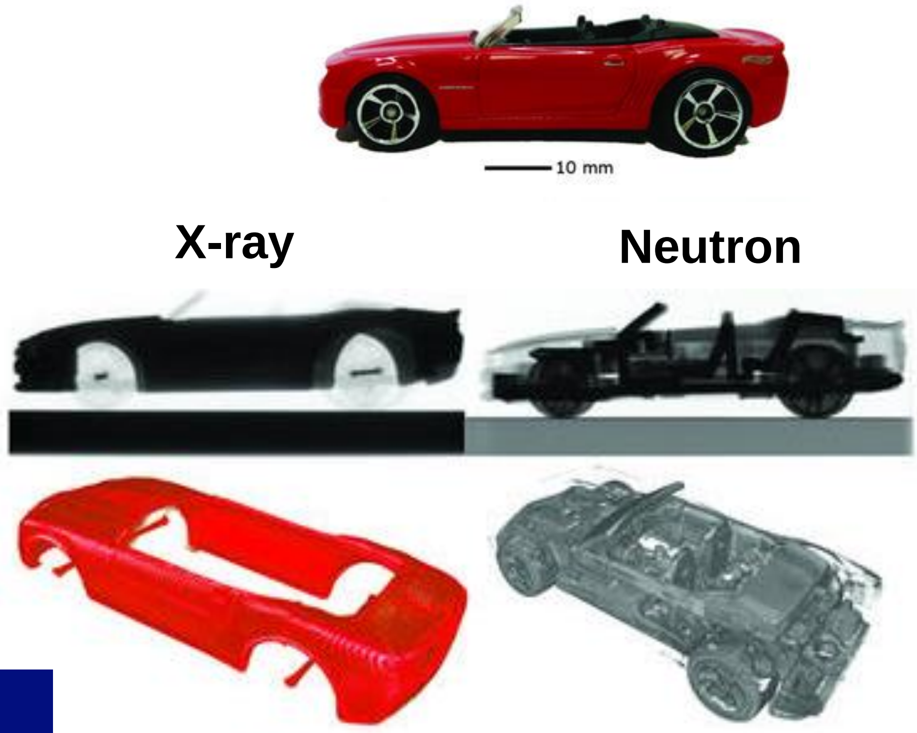
Industry:
Corky Mittelsteadt (Plug)
Kathy Ayers (NEL)
Andrew Smeltz (DeNora)
Udit Shrivastava (Cummins)
Andrew Park (Chemours)

University:
Svitlana Pylypenko (CSM)
Iryna Zenyuk (UCI)

Neutron Imaging

Comparison of the relative size of the x-ray and neutron scattering cross section for various elements.



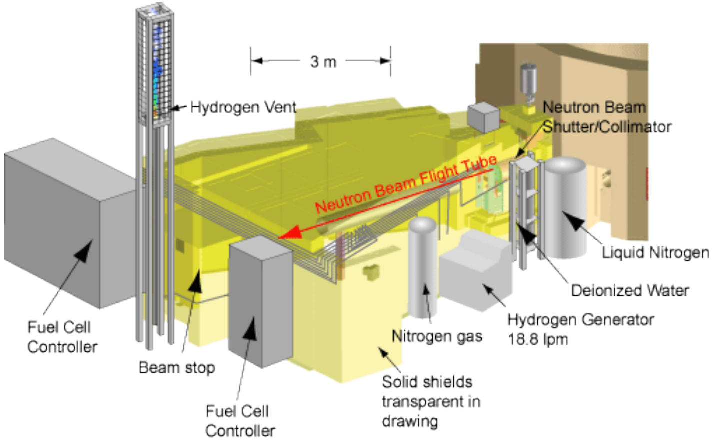


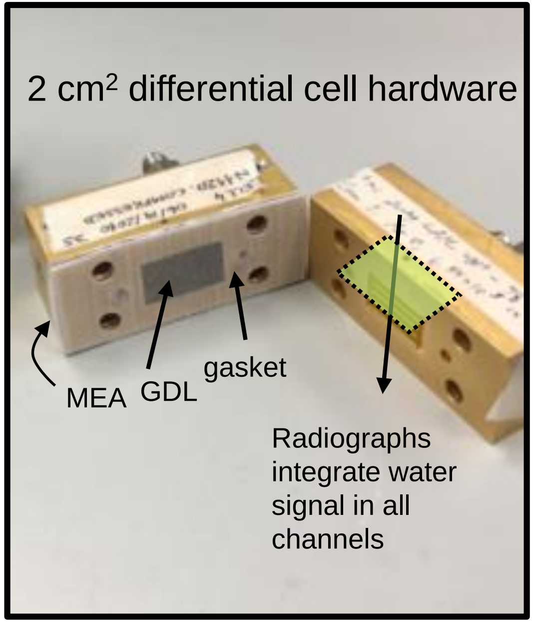
Neutrons are an excellent probe for hydrogen in metal since metals can have a much smaller cross section to neutrons compared to hydrogen.

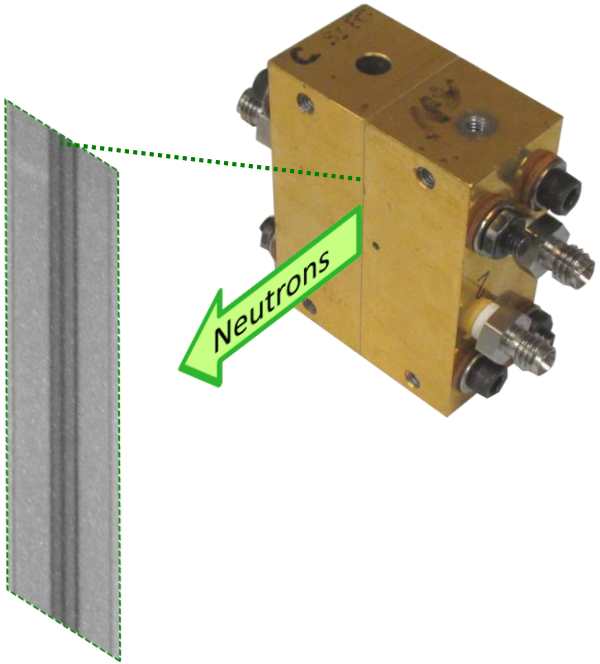
https://www.nist.gov/news-events/news/2017/11/nists-next-trick-will-fill-your-eyes-double-vision

Water Imaging using Neutrons

NIST Neutron Imaging Facility

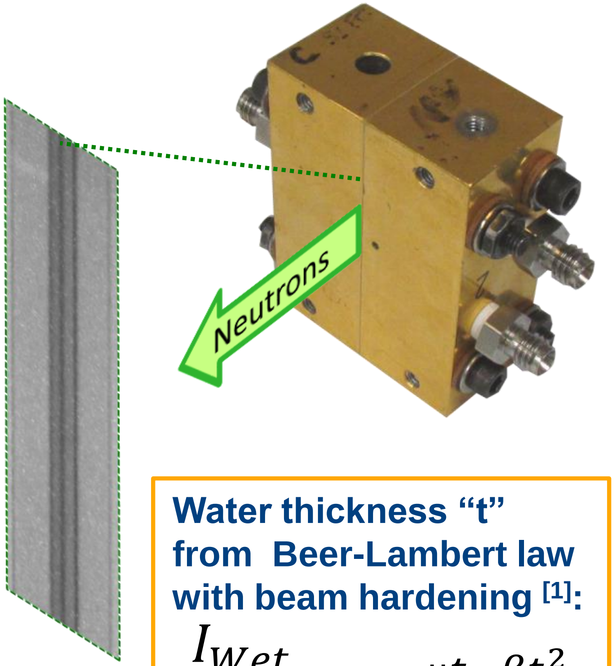




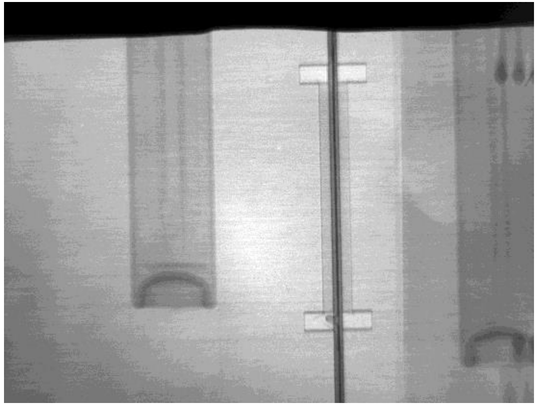


- Neutron radiography is a powerful technique for imaging water saturation and distribution in electrolyzer cells
- LANL has developed multiple differential and integral cell hardware designs for operando water imaging in fuel cells and electrolyzers

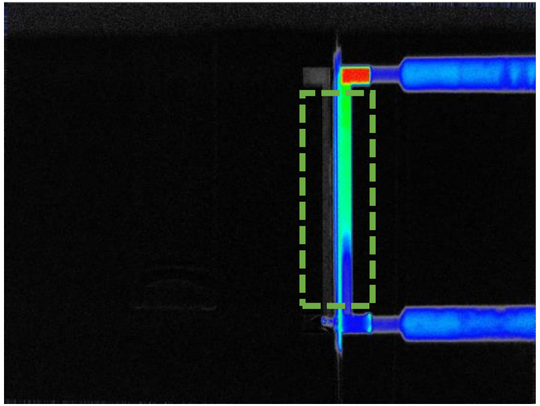
Water Thickness Estimation



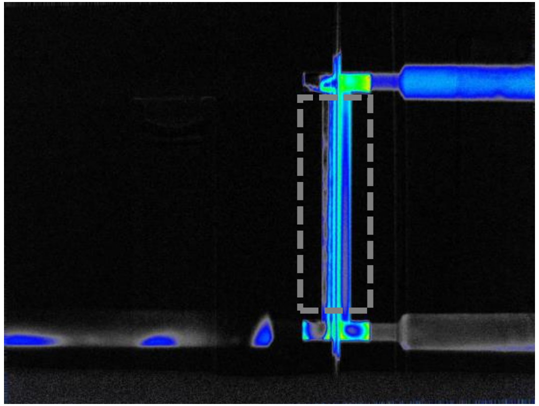
Dry

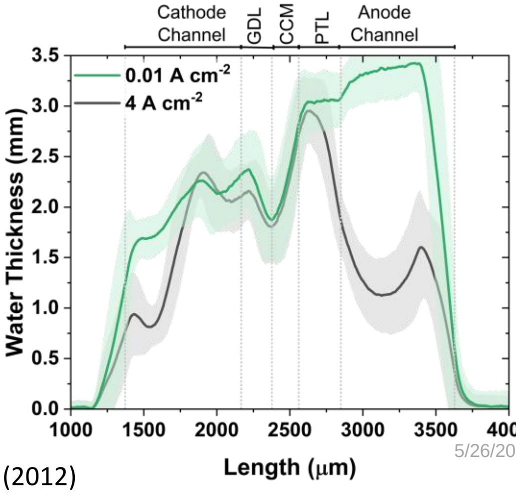


0.01 A cm^{-2}



4 A cm^{-2}



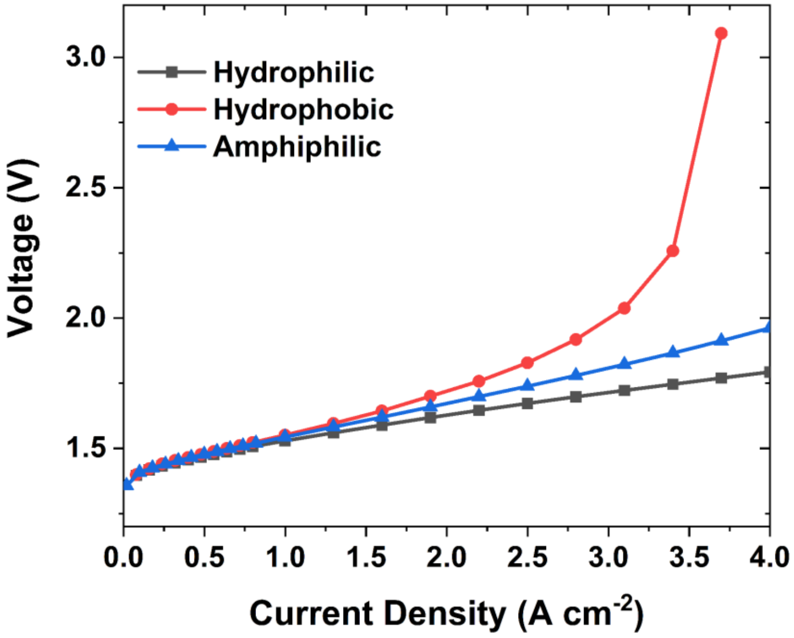


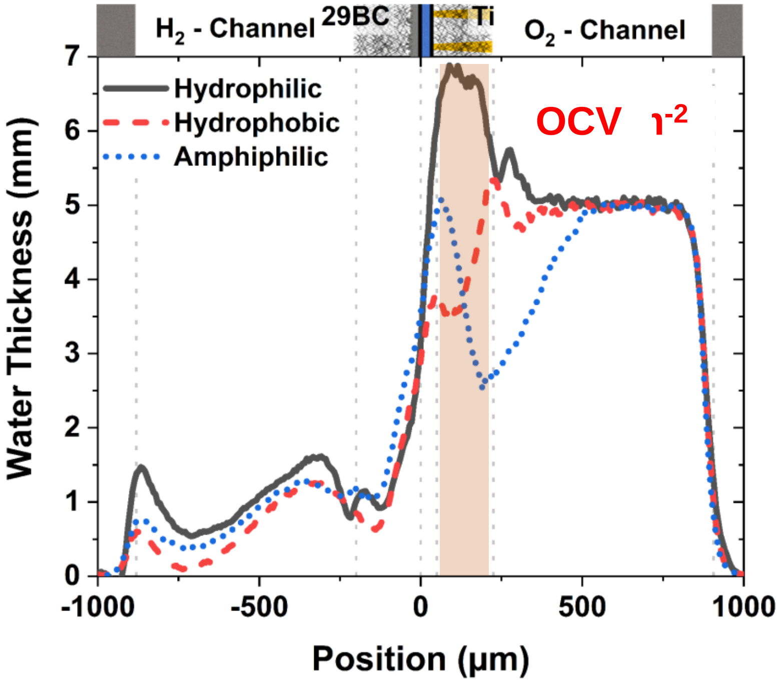
Water thickness "t" from Beer-Lambert law with beam hardening [1]:

$$\frac{I_{Wet}}{I_{Dry}} = e^{-\mu t - \beta t^2}$$

[1] Hussey et al, *Journal of Applied Physics* 112 (10), 104906 (2012)

Effect of Porous Transport Layer Wettability





- LANL has used neutron radiography to relate changes in electrolyzer performance to changes in water content for anode PTLs with hydrophobic and hydrophilic treatments
- LANL experience and capabilities can be used to support electrolyzer development work throughout the consortium

Thank You

Questions?

Structured Electrodes for Energy Conversion, Energy Storage, and Ionic Separations

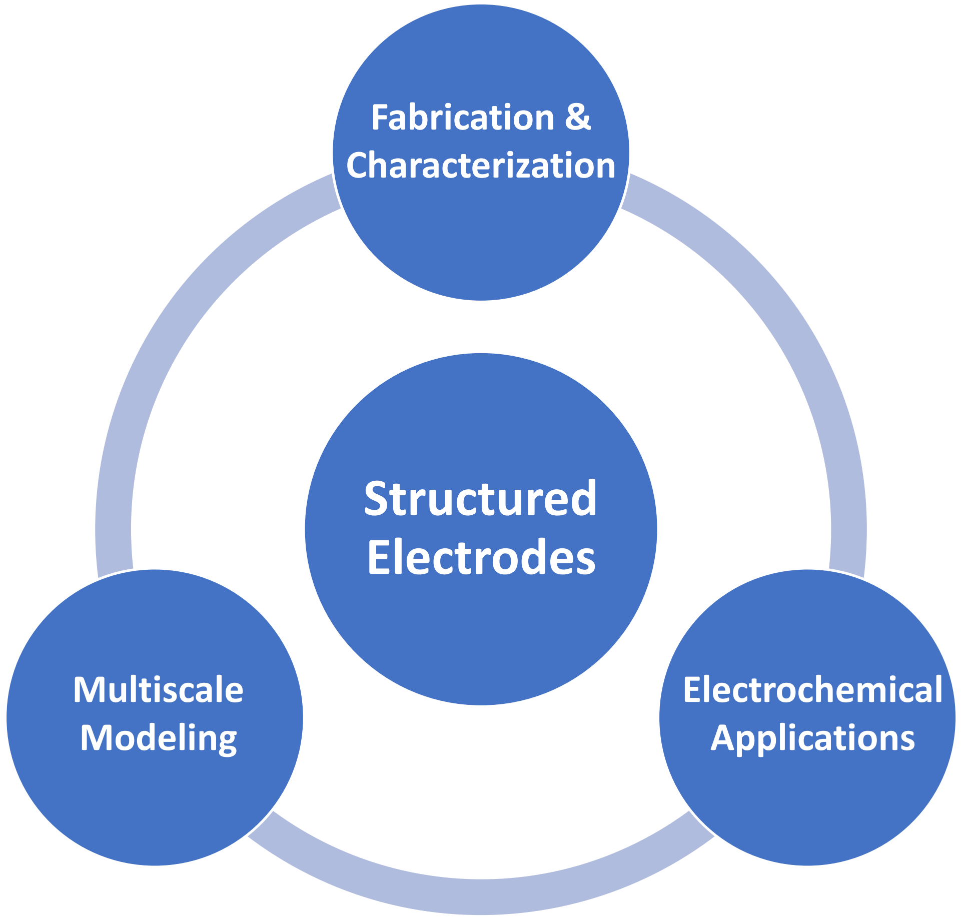
MPA-11: Rod Borup, Jerzy Chlistunoff, Ana Dibert, George Goff, Alex Gupta, Siddharth Komini Babu, Chung Hyuk Lee, Wipula Liyanage, Ulises Martinez, Luigi Osmieri, Jacob Spendelow, Xiaojing Wang, Gaoqiang Yang

MPA-CINT: Jinkyoung Yoo, Yeonhoo Kim

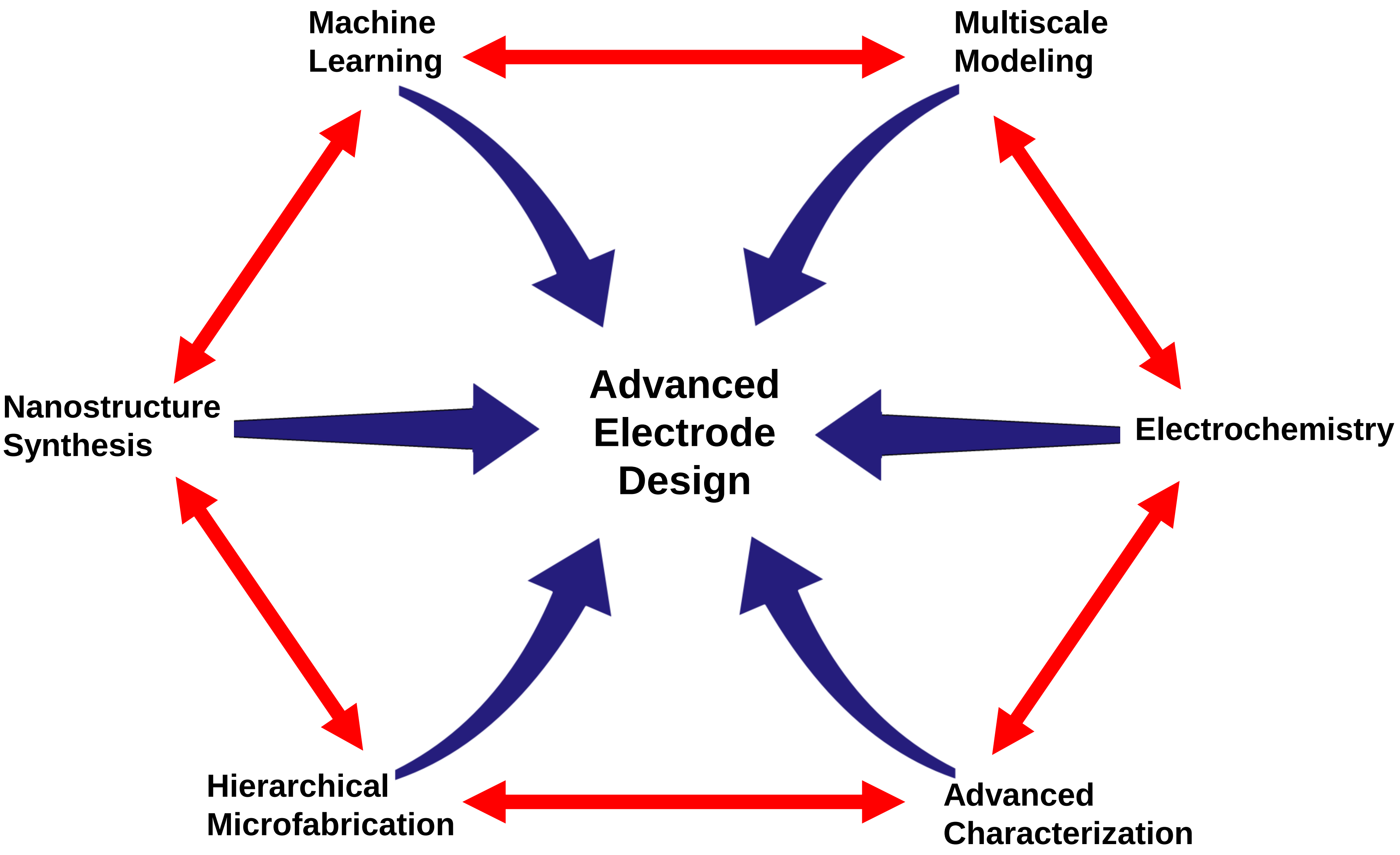
MST-7: Brian Patterson, Ethan Walker, Steven Young

T-4: Towfiq Ahmed, Ayhan Duzgan, Alper Ince, Hasnain Hafiz, Mohammad Karim, Wilton Kort-Kamp, Azimur Rahman, Mustafa Fazil Serincan

SIGMA-2: Ted Holby



Advanced Electrode Design Capabilities

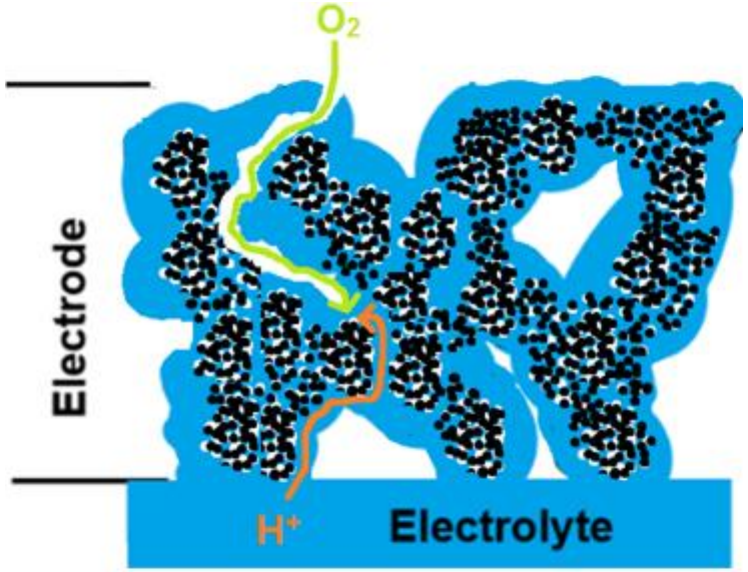


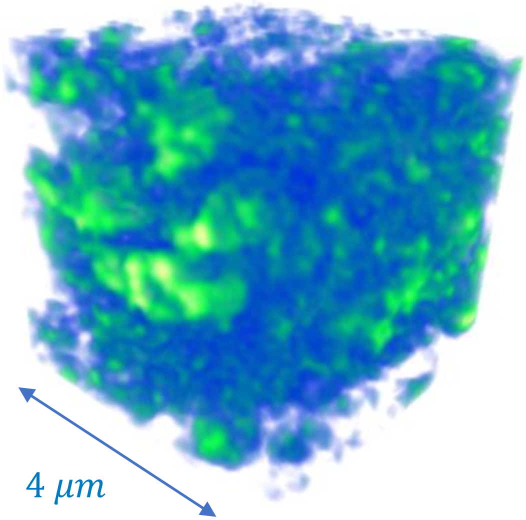
What is a Structured Electrode?

Three key attributes:

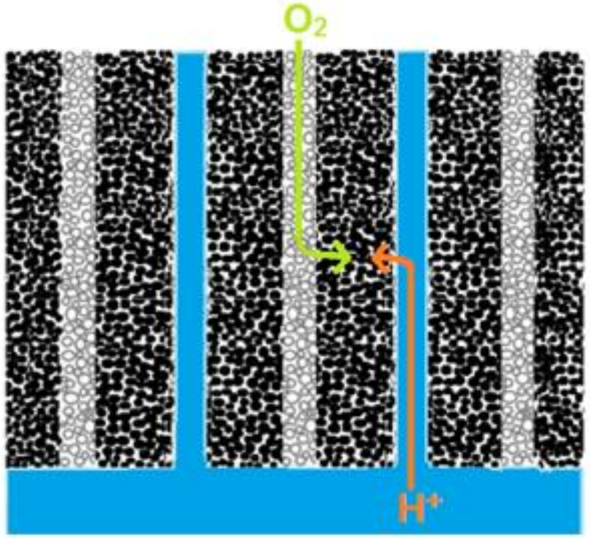
1. **Differentiated.** Different electrode functions are separated into different segments, enabling each segment to be optimized for its specific function
2. **Ordered.** Ordered arrays of straight-through transport channels reduce tortuosity and non-percolation
3. **Hierarchical.** Control of structural features on multiple length scales is used to maximize transport rates and interfacial area

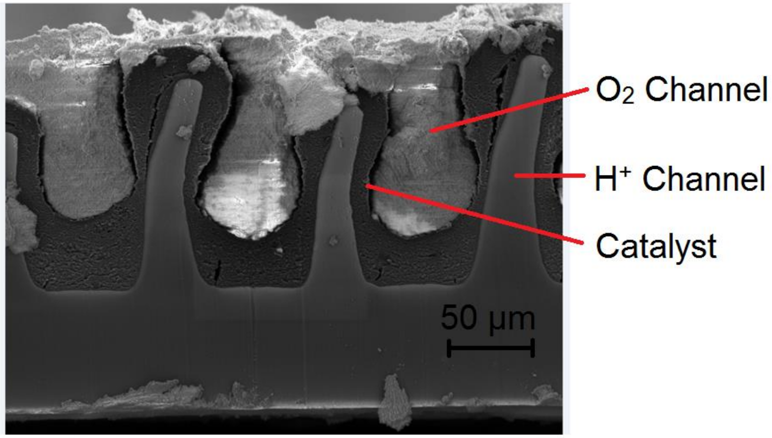
Conventional Electrode



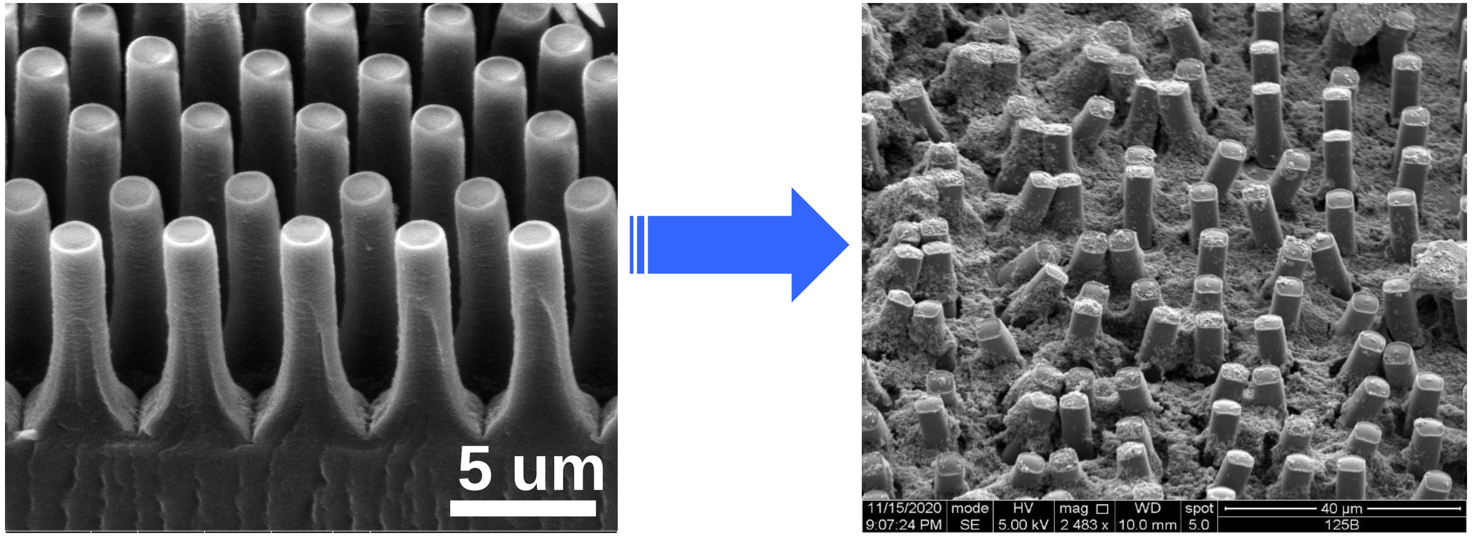


Structured Electrode



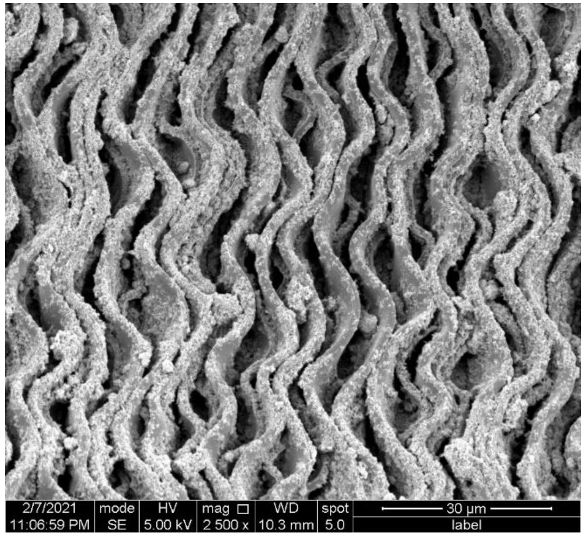


Progress in Array Electrode Fabrication

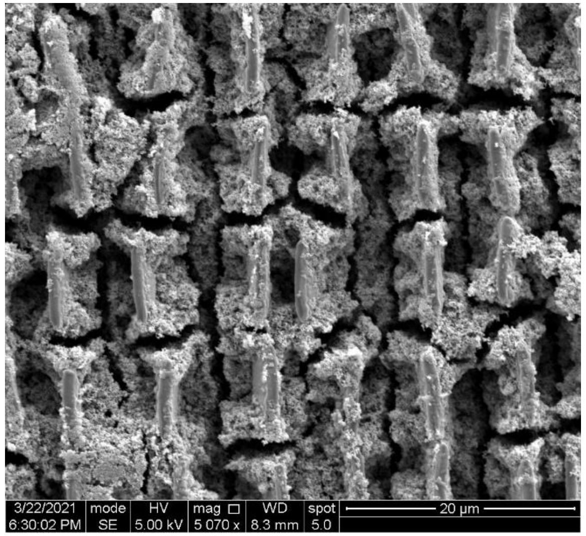


Plus-shape pattern provides robust support without pillar collapse

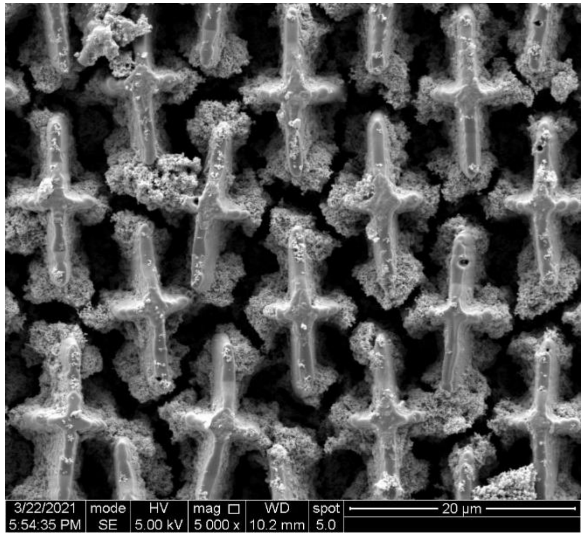
Ridge



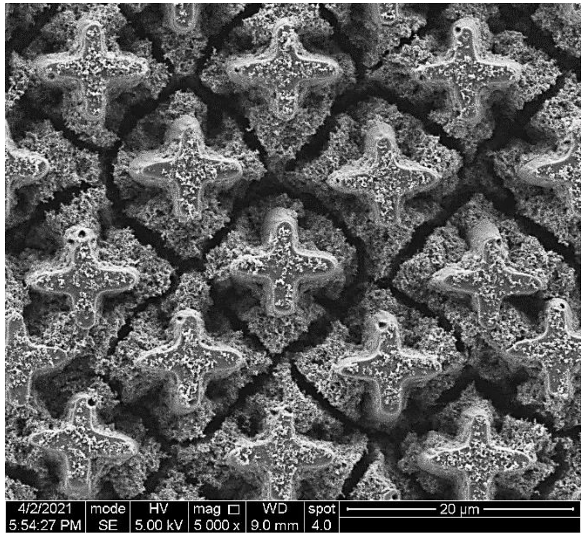
Dash



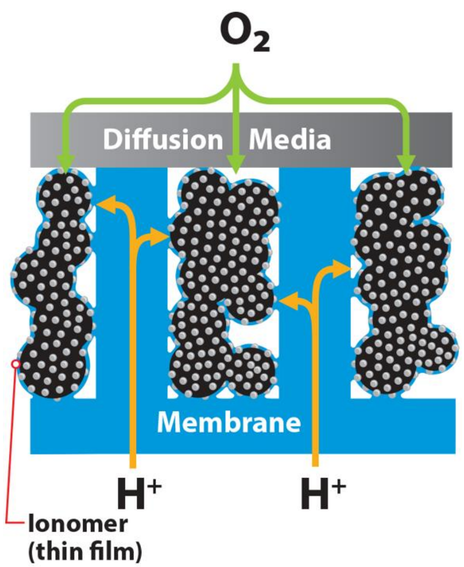
Cross

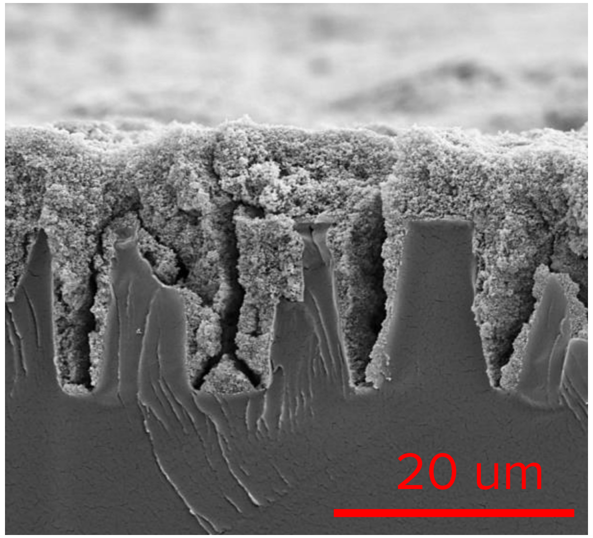


Plus

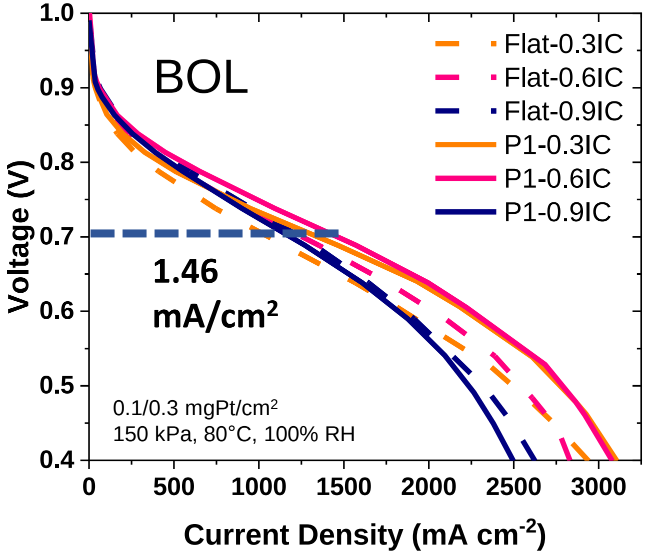


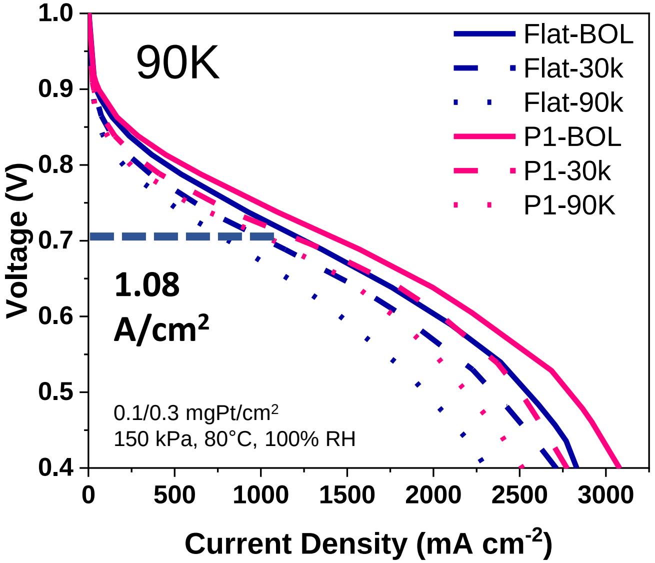
Array electrodes

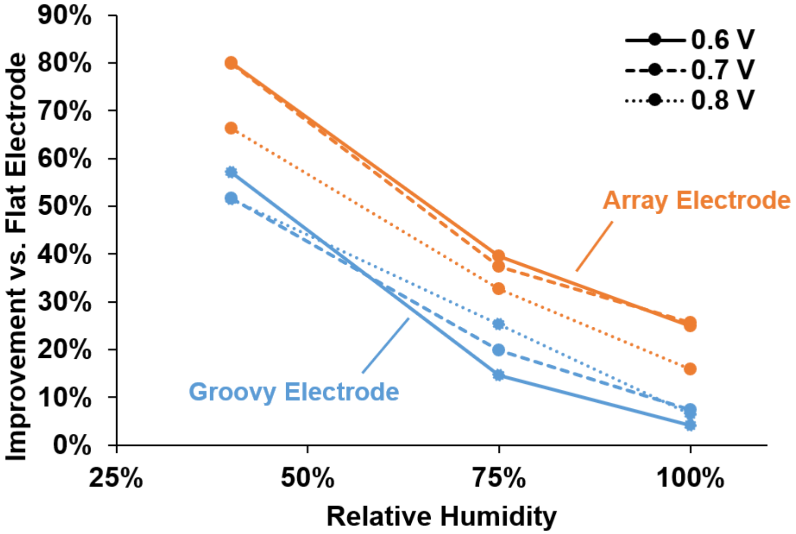




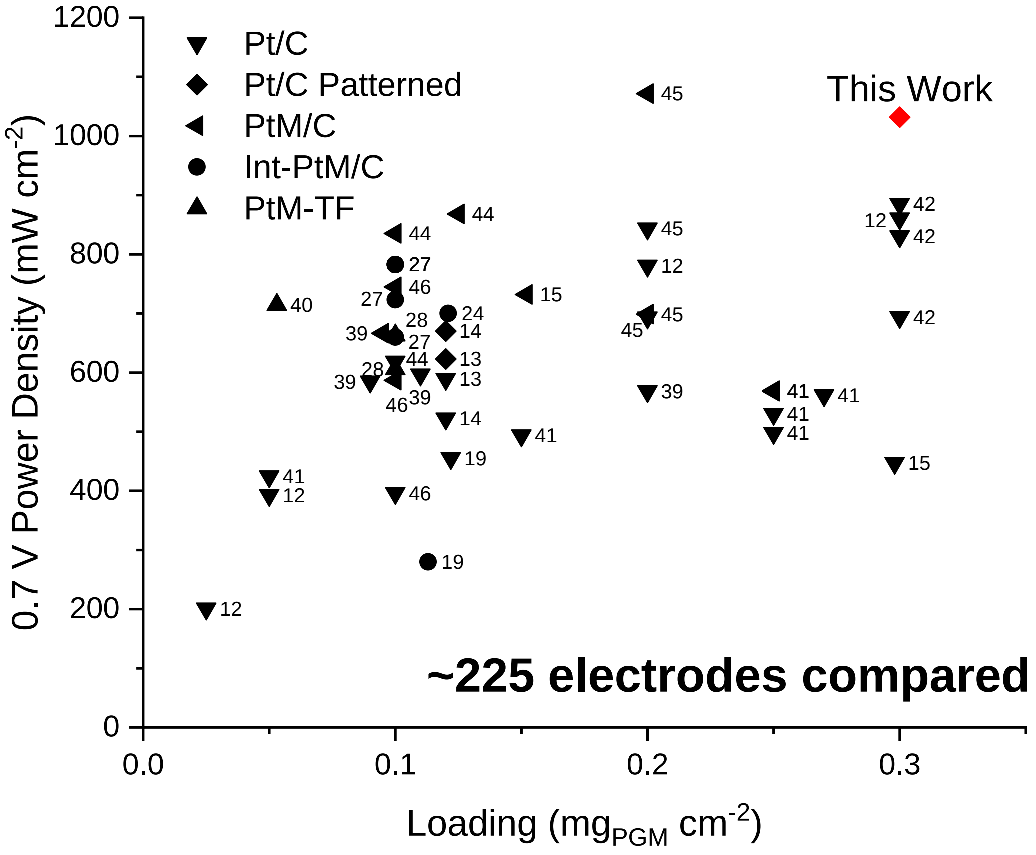
- Non-tortuous ionomer channels provide H^+ highways
- Lower I/C enhances O_2 transport
- Advanced electrode structures provide up to 80% higher power

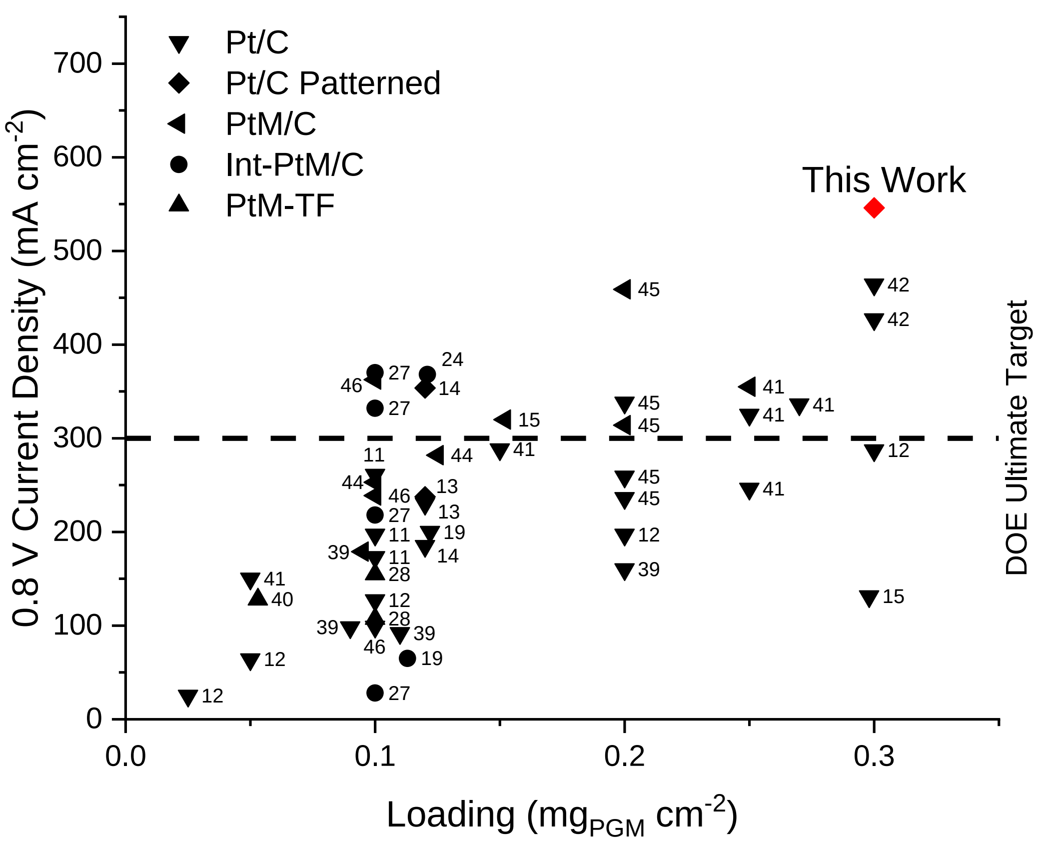






Array Electrode Performance





Array electrodes with Pt/C outperform even advanced Pt alloys